Supporting Information

M-M Bond-Stretching Energy Landscapes for $M_2(dimen)_4^{2+}$ (M = Rh, Ir; dimen = 1,8-diisocyanomenthane) Complexes

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S-1: Determining Thermodynamic Parameters for Isomer Equilibration

To determine the thermodynamic parameters for the equilibrium between the two isomers, absorption spectra at various temperatures are deconvoluted and the oscillator strengths[1] (which are proportional to the area under the curve for each absorption band) are determined. In order to properly describe the absorption spectra of $Ir_2(dimen)_4^{2+}$ over the entire temperature range of this study (30-296 K) a minimum of four Gaussian curves are required. This approach is designed to give an approximation of the true band structure of the complex as a function of temperature. These Gaussian curves (G_1-G_4) have maxima at 16,600, 18,260, 19,920, and 21,270 cm^{-1} (Figure S1).

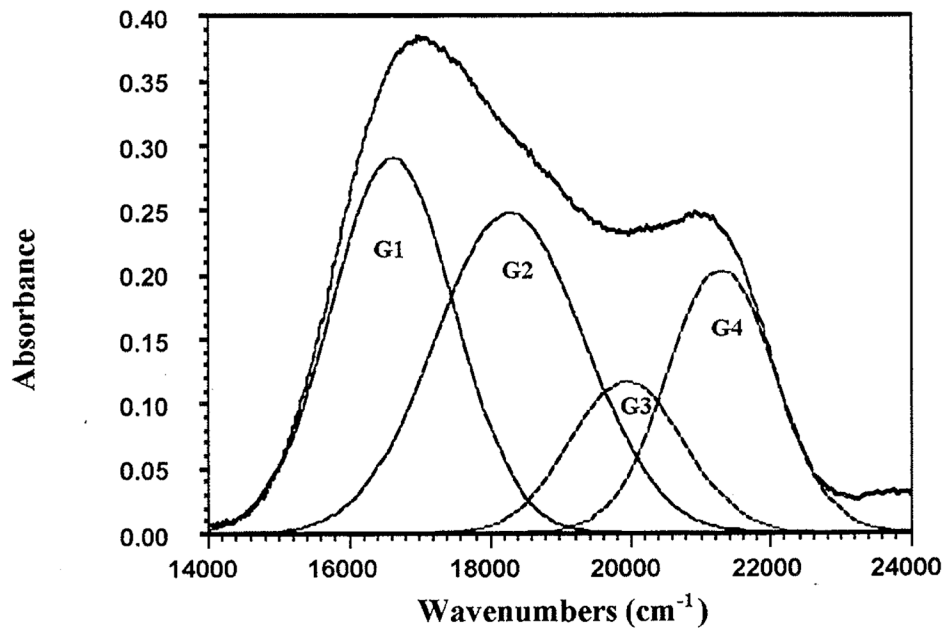

Figure S1: Gaussian curve fit (G_1-G_4) of the electron absorption spectra of $Ir_2(dimen)_4^{2+}$ at 296 K. G_1 and G_2 are assigned to the band at 17,241 cm^{-1} (580 nm) and G_3 and G_4 to the 21,277 cm^{-1} (470 nm) band.

The oscillator strength for G_3 and G_4 decreases as the temperature is dropped from 296 K to 120 K, with both maintaining the same absorption maximum. The G_3+G_4 absorption profile resembles the solid-state absorption spectrum of $[Ir_2(dimen)_4^{2+}](PF_6)_2$ (long Ir-Ir separation, eclipsed ligand conformation) which has a maximum at 21,370 cm^{-1} with a shoulder at 19,460 cm^{-1}. Over the same temperature range, the G_1 oscillator strength increases while its maximum remains constant. The G_2 Gaussian, however, decreases in oscillator strength and the absorption maximum red-shifts from 18,260 cm^{-1} to 17,900 cm^{-1}. This large shift in the absorption maximum for G_2 suggests that it does not represent another isomer of the complex; rather, the absorption profile described by G_1+G_2 is asymmetric and sharpens as the temperature is lowered. This resembles the solid-state absorption spectrum of $[Ir_2(dimen)_4^{2+}][B(C_6H_5)_4]_2$ (short Ir-Ir separation, twisted ligand conformation) which has an absorption maximum at 17,241 cm^{-1} with a shoulder at 20,040 cm^{-1}. Based on the resemblance of G_1+G_2 to the $B(C_6H_5)$ salt and G_3+G_4 to the PF_6 salt, it is proposed that G_1+G_2 describe the short isomer and G_3+G_4 describe the long isomer.

$$\text{Long} \rightleftharpoons \text{Short} \qquad \text{(Eqn. 1)}$$

$$K = \frac{G_1 + G_2}{G_3 + G_4} \qquad \text{(Eqn. 2)}$$

$$\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ = -RT \ln K \qquad \text{(Eqn. 3)}$$

$$\ln K = \left(-\frac{\Delta H^\circ}{R}\right)\frac{1}{T} + \frac{\Delta S^\circ}{R} \qquad \text{(Eqn. 4)}$$

From the oscillator strengths, it is possible to determine the equilibrium constant between the short and long isomer (Eqn. 1). From the temperature dependent absorption studies, the ratio of G_1+G_2 to G_3+G_4 gives the equilibrium constant, K (Eqn. 2), at a given temperature. A van't Hoff plot (Eqns. 3&4, Figure S2) of ln(K) *vs*. 1/T gives thermodynamic parameters ΔH° = -800 cal/mol and ΔS° = 1.44 cal mol^{-1} K^{-1}. This indicates that the short isomer is ~ 0.8 kcal/mol lower in energy than the long form.

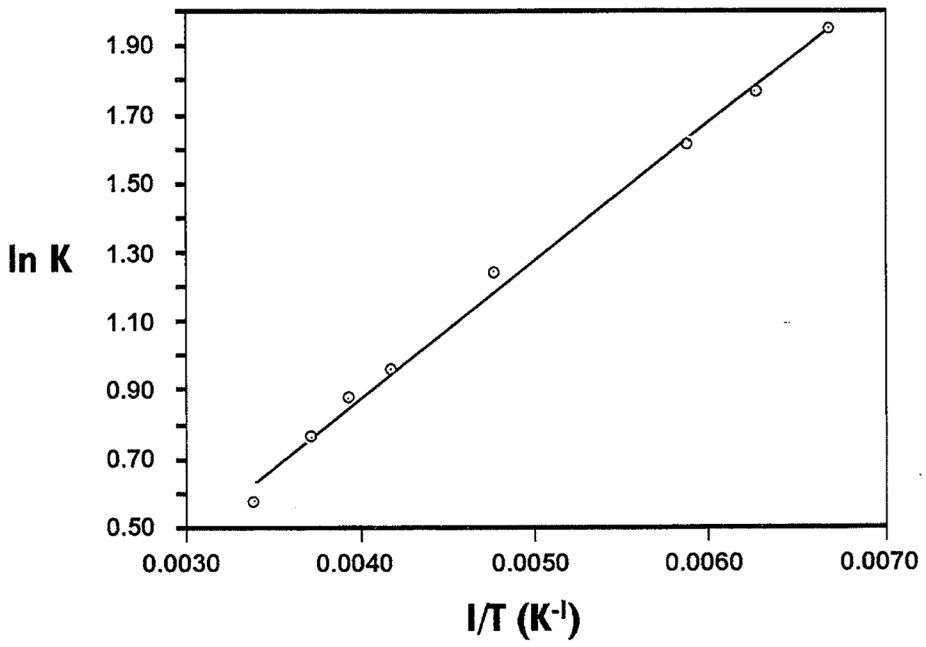

Figure S2: Van't Hoff plot based on the calculated oscillator strengths. ΔH° and ΔS° are -798.8 cal mol^{-1} and 1.441 cal mol^{-1} K^{-1}, respectively.

S-2: Ligand Calculations

A relaxed potential-energy surface scan was carried out in *Gaussian03* using the ligand geometry seen in Figure S3:

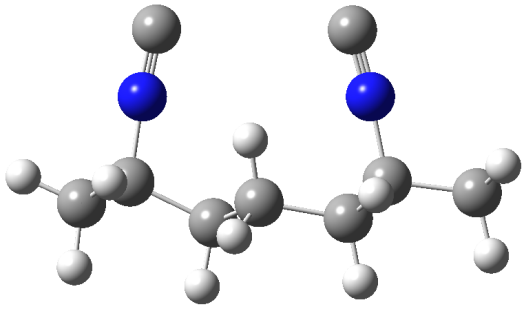

Figure S3: Starting ligand geometry used for DFT calculations

The route section was:

```
# opt=modredundant b3lyp/6-311g geom=connectivity
```

The ModRedundant section was:

```
B    1   14 3.8000 S  40 0.0250
D    1    5   11   14 0.0000 S  20 1.0000
```

This section requests a relaxed potential-energy scan—that is, a geometry optimization is performed at every step—with the distance between the two terminal carbon atoms of the isonitrile groups (the "bridging C---C" distance) starting at 3.8 Å and being increased by 0.025 Å for 40 iterations. At the same time, the twist angle (defined as the C(terminal)—C(backbone)—C(backbone')—C(terminal') dihedral angle) was scanned from 0° to 20° in 1° increments. This corresponds to 41*21=861 different geometries that were optimized.[2]

The energies (Figure S4) were exported, converted to kcal/mol from Hartrees, and multiplied by 4 to include the entire ligand set.

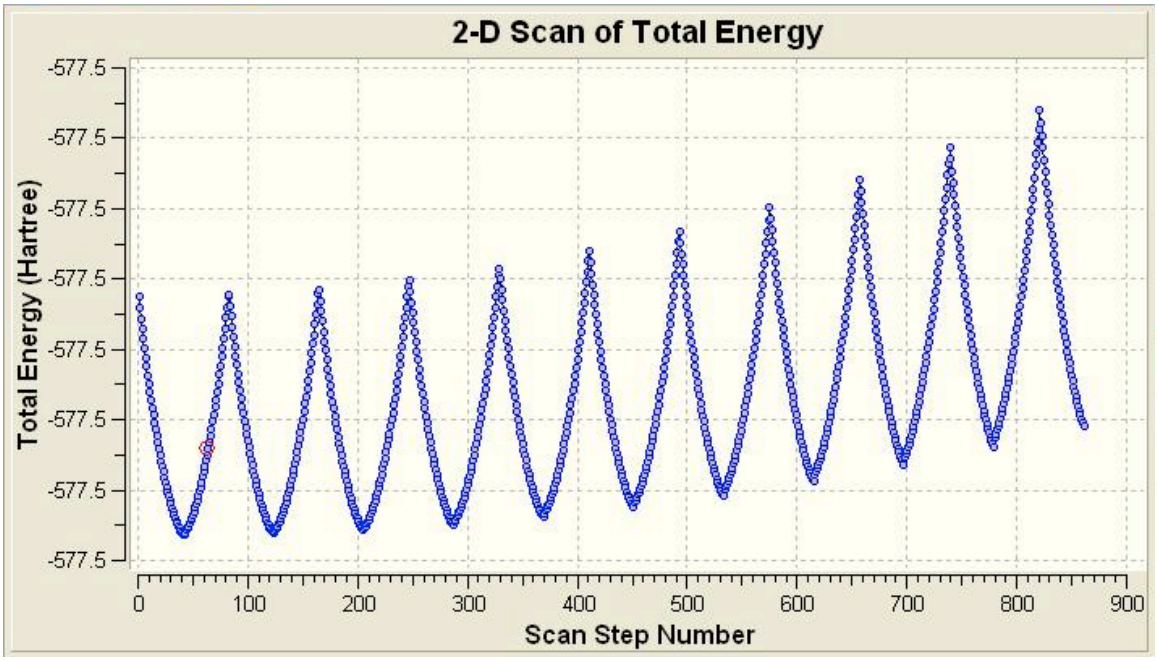

Figure S4: Optimized geometry energies (in Hartrees) for the 861 ligand structures examined by DFT potential-energy surface scan. (Note: the program scans all C---C distances at a single twist angle before increasing the angle and repeating the process; this gives rise to the periodic shape observed in this "energy *vs*. step number" plot.)

S-3: Measuring the Metal-Metal Distance

In order to (1) plot the potential-energy curves and surfaces and (2) calculate the appropriate Morse interaction for a given structure, the effective metal-metal separations were measured from the optimized-ligand geometries. An iridium atom was manually added (Figure S5) 1.93 Å away from each of the terminal isonitrile carbon atoms (the iridium atoms were placed linearly to the isonitrile C-N). The Ir-Ir separation for each structure was then measured.

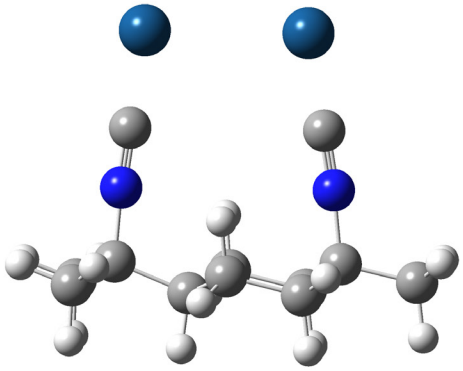

Figure S5: Iridium atoms were added manually to the optimized ligand geometries at distances of 1.93 Å from the terminal C atoms and with N-C-Ir bond angles of 180°.

S-3: Measuring the Out-of-Plane Angle

The A_{2u} distortional energy depends on the magnitude of the angle by which the metal centers are distorted out of plane, ϕ. In order to quantify this, a C-Ir-Ir "bond" angle, θ, was measured for each of the optimized ligand geometries (Figure S6). Using basic geometry we see that θ-90 (90-θ in the case of θ<90°) corresponds to one-half of ϕ, the out-of-plane distortional angle (Figure S7). Because the ligands are asymmetric, the same angle, θ, was measured for every structure (shown in the figure). Finally, ϕ is plugged into equation 5 to obtain the A_{2u} out-of-plane distortional energy. (Note: the value, E_{A2u}, from Eqn. 5 is doubled to obtain the total distortional energy for *two* square-planar distortions.)

$$E_{A2u} = F\phi^2 \qquad \text{(Eqn. 5)}$$

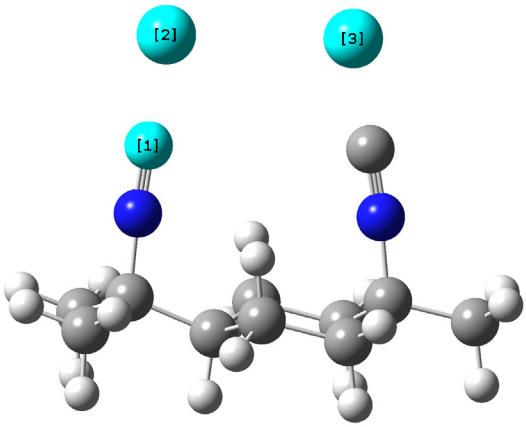

Figure S6: The angle **[1]-[2]-[3]** was measured from each optimized ligand structure (with iridium atoms added manually). Because the ligand is asymmetric, it was always oriented in the way shown in the figure.

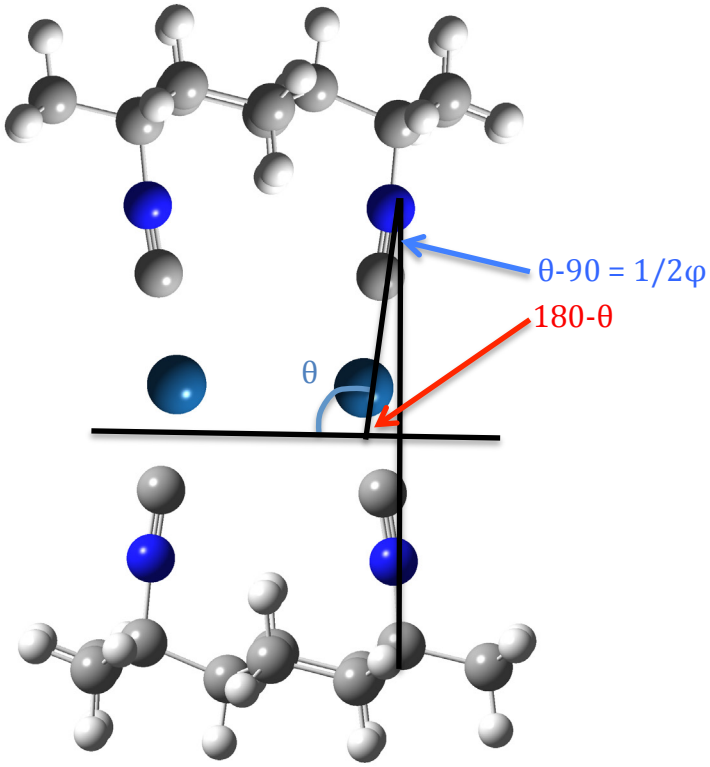

Figure S7: The relationship between the C-Ir-Ir "bond" angle, θ, and the out-of-plane angle, ϕ. In the case where θ>90°, θ-90 is equal to one-half of the out-of-plane distortion of each metal center (this is due to the fact that the ligand opposite is identically out of plane). For θ>90°, the relationship is 1/2ϕ = 90-θ.

S-4: Electronic Excited State Predicted Surface

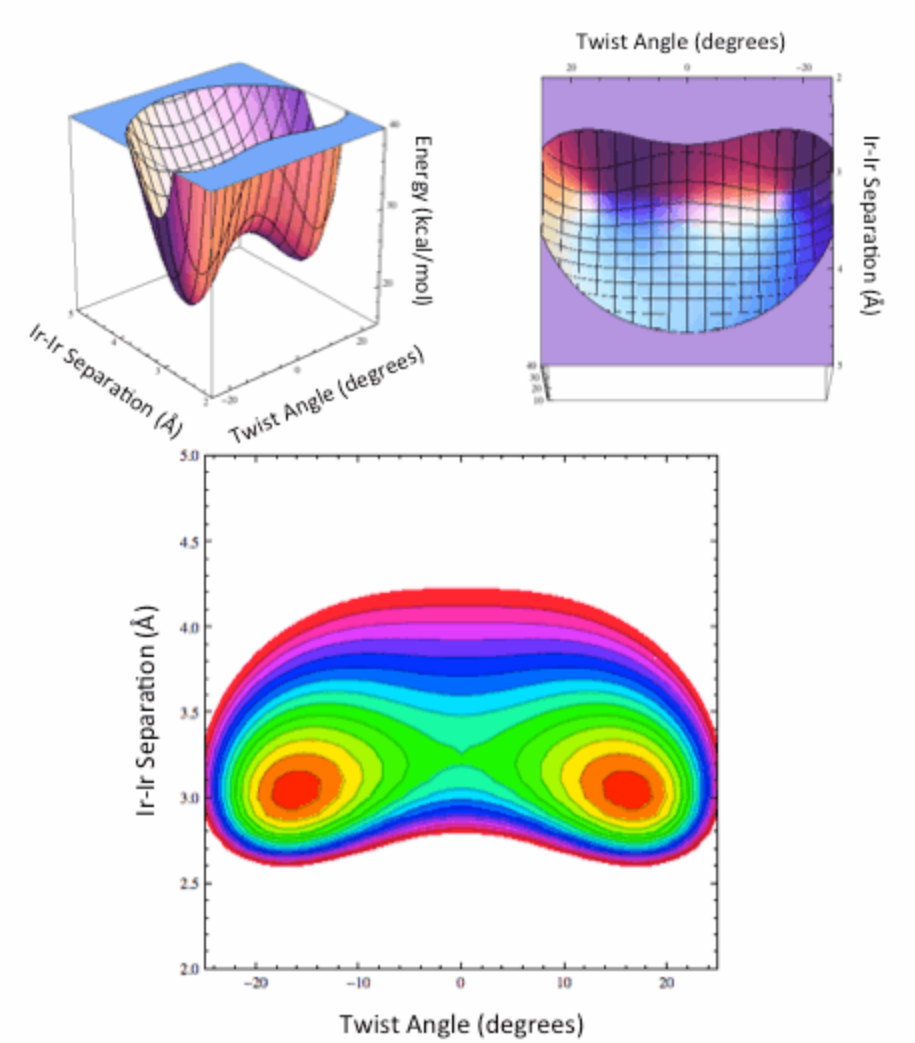

Figure S8: Calculated potential energy surface for the triplet electronic-excited state of $[Ir_2(dimen)_4]^{2+}$. Contour spacing is 1 kcal/mol. We observe a single minimum along the Ir-Ir coordinate, corresponding to an Ir-Ir distance of 3 Å and a dihedral twist angle of ± 16°. ($R_{e,Ir\text{-}Ir}$=2.87 Å, $F_{Ir\text{-}Ir}$=0.99 mdyne/Å, well-depth estimated to be 50 kcal/mol).

S-5: Potential-Energy Curve and Surface Data

Table S1: Structural Data and Energy Calculations

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
1	3.800	0	3.20516	97.588	-577.519257478	8.464596913	0.029640783	13.11930946	21.61354716
2	3.825	0	3.24888	97.335	-577.519409609	8.082742626	0.015979637	12.259043	20.35776526
3	3.850	0	3.29329	97.093	-577.519558007	7.710258304	0.16752873	11.46347404	19.34126107
4	3.875	0	3.33791	96.841	-577.519702421	7.347773965	0.454584726	10.66339539	18.46575408
5	3.900	0	3.38251	96.597	-577.519842912	6.995136497	0.848267516	9.916291851	17.75969586
6	3.925	0	3.42721	96.352	-577.519979452	6.652416182	1.325965166	9.193424438	17.17180579
7	3.950	0	3.47204	96.100	-577.520112062	6.319560308	1.868367668	8.478440995	16.66636897
8	3.975	0	3.51688	95.858	-577.520240735	5.996586446	2.457290797	7.81906938	16.27294662
9	4.000	0	3.56191	95.603	-577.520365549	5.683298812	3.081095776	7.153154032	15.91754862
10	4.025	0	3.60698	95.349	-577.520486521	5.379654737	3.726029746	6.519308426	15.62499291
11	4.050	0	3.65215	95.095	-577.520603734	5.085445888	4.383167062	5.914863256	15.38347621
12	4.075	0	3.69738	94.839	-577.520717268	4.80047146	5.04386995	5.335407271	15.17974868
13	4.100	0	3.74268	94.582	-577.520827210	4.524513082	5.701691812	4.783728262	15.00993316
14	4.125	0	3.78804	94.324	-577.520933642	4.257364931	6.35115541	4.260177581	14.86869792
15	4.150	0	3.83346	94.065	-577.521036647	3.998818673	6.988004539	3.765107945	14.75193116
16	4.175	0	3.87894	93.804	-577.521136301	3.748683545	7.608894491	3.2971397	14.65471774
17	4.200	0	3.92446	93.543	-577.521232675	3.506781336	8.21099104	2.860214716	14.57798709
18	4.225	0	3.97002	93.281	-577.521325829	3.272961442	8.792397886	2.452837588	14.51819692
19	4.250	0	4.01563	93.018	-577.521415810	3.047105893	9.351886157	2.075366504	14.47435855
20	4.275	0	4.06126	92.753	-577.521502650	2.829134367	9.888202148	1.726906224	14.44424274
21	4.300	0	4.10692	92.487	-577.521586362	2.619014233	10.40097088	1.409314443	14.42929956
22	4.325	0	4.15261	92.220	-577.521666954	2.416725412	10.89000259	1.122954813	14.42968282
23	4.350	0	4.19831	91.952	-577.521744428	2.222262883	11.35516202	0.868192358	14.44561726
24	4.375	0	4.24404	91.683	-577.521818792	2.035606566	11.79693517	0.645393466	14.4779352
25	4.400	0	4.28978	91.412	-577.521890064	1.85671128	12.21557302	0.454282205	14.52656651
26	4.425	0	4.33553	91.140	-577.521958262	1.685531845	12.61166133	0.296118837	14.59331201
27	4.450	0	4.38131	90.866	-577.522023412	1.522002999	12.98604086	0.170880347	14.6789242
28	4.475	0	4.42710	90.592	-577.522085544	1.366049442	13.33928766	0.079854564	14.78519167
29	4.500	0	4.47291	90.316	-577.522144688	1.217595873	13.67227689	0.022752572	14.91262533
30	4.525	0	4.51875	90.039	-577.522200876	1.07656197	13.98590022	0.000346566	15.06280875
31	4.550	0	4.56463	89.760	-577.522254140	0.942867413	14.28105353	0.013124381	15.23704532
32	4.575	0	4.61054	89.480	-577.522304506	0.81644694	14.55851004	0.061611675	15.43656865
33	4.600	0	4.65649	89.199	-577.522351998	0.69724031	14.81916858	0.146191245	15.66260014
34	4.625	0	4.70249	88.916	-577.522396638	0.585192303	15.06390673	0.267741009	15.91684004
35	4.650	0	4.74853	88.632	-577.522438440	0.480267778	15.29347991	0.426411125	16.20015881
36	4.675	0	4.79463	88.347	-577.522477412	0.382446655	15.50877492	0.622589854	16.51381143
37	4.700	0	4.84078	88.060	-577.522513557	0.291721404	15.71050713	0.857550673	16.85977921
38	4.725	0	4.88699	87.771	-577.522546874	0.208094535	15.89945962	1.132078308	17.23963247
39	4.750	0	4.93325	87.481	-577.522577356	0.131583617	16.07630571	1.445814803	17.65370413
40	4.775	0	4.97957	87.190	-577.522604994	0.062211242	16.24177127	1.799156623	18.10313913

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)^3**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
41	4.800	0	5.02594	86.897	-577.522629779	0	16.39648042	2.193915433	18.59039585
42	4.800	1	5.02651	86.850	-577.522625944	0.009625988	16.39831693	2.260879623	18.66882254
43	4.775	1	4.97980	87.181	-577.522601099	0.071987833	16.24256507	1.810699926	18.12525283
44	4.750	1	4.93353	87.474	-577.522573392	0.1415334	16.07734011	1.453861461	17.67273497
45	4.725	1	4.88728	87.763	-577.522542848	0.21819994	15.90060584	1.14021907	17.25902485
46	4.700	1	4.84107	88.051	-577.522509468	0.301984941	15.71173283	0.865525785	16.87924355
47	4.675	1	4.79493	88.337	-577.522473256	0.392878365	15.51013	0.630145487	16.53315385
48	4.650	1	4.74884	88.622	-577.522434216	0.49087017	15.29497545	0.432667991	16.21851362
49	4.625	1	4.70280	88.906	-577.522392344	0.595970398	15.065503	0.272703666	15.93417707
50	4.600	1	4.65680	89.189	-577.522347632	0.708199127	14.8208712	0.149864249	15.67893457
51	4.575	1	4.61086	89.470	-577.522300067	0.82758899	14.56038322	0.064004141	15.45197635
52	4.550	1	4.56496	89.749	-577.522249629	0.954190185	14.28311068	0.014355019	15.25165588
53	4.525	1	4.51910	90.028	-577.522196292	1.088067976	13.98822168	0.000178637	15.0764683
54	4.500	1	4.47326	90.305	-577.522140028	1.229292641	13.6747446	0.021196102	14.92523334
55	4.475	1	4.42746	90.580	-577.522080809	1.377934463	13.34198297	0.076650028	14.79656746
56	4.450	1	4.38168	90.854	-577.522018603	1.534073762	12.98897918	0.166177444	14.68923038
57	4.425	1	4.33592	91.127	-577.521953379	1.69778835	12.61494243	0.289403757	14.60213454
58	4.400	1	4.29018	91.399	-577.521885107	1.869153528	12.21913326	0.445955743	14.53424253
59	4.375	1	4.24445	91.669	-577.521813763	2.048229537	11.8007901	0.634700741	14.48372038
60	4.350	1	4.19875	91.939	-577.521739326	2.235069086	11.35952489	0.856666828	14.45126081
61	4.325	1	4.15305	92.207	-577.521661782	2.429707318	10.89459513	1.109841597	14.43414405
62	4.300	1	4.10739	92.473	-577.521581122	2.632166822	10.40612401	1.393492273	14.4317831
63	4.275	1	4.06174	92.739	-577.521497344	2.842452618	9.893717464	1.709386999	14.44555708
64	4.250	1	4.01612	93.003	-577.521410440	3.060584786	9.357770948	2.054787885	14.47314362
65	4.225	1	3.97053	93.266	-577.521320397	3.286595958	8.798780665	2.430461203	14.51583783
66	4.200	1	3.92498	93.528	-577.521227182	3.520568964	8.217749641	2.836047399	14.574366
67	4.175	1	3.87948	93.789	-577.521130749	3.762619265	7.61615476	3.271188288	14.64996231
68	4.150	1	3.83402	94.049	-577.521031037	4.012899975	6.99575773	3.73552705	14.74418475
69	4.125	1	3.78861	94.307	-577.520927976	4.271586795	6.359238881	4.226745272	14.85757095
70	4.100	1	3.74326	94.564	-577.520821490	4.538870488	5.710064592	4.746217142	14.99515222
71	4.075	1	3.69798	94.821	-577.520711496	4.814959388	5.052621385	5.295788047	15.16336882
72	4.050	1	3.65276	95.076	-577.520597907	5.100071867	4.392076184	5.870830731	15.36297878
73	4.025	1	3.60762	95.330	-577.520480640	5.394416259	3.735286268	6.473076656	15.60277918
74	4.000	1	3.56255	95.582	-577.520359612	5.698200896	3.090135442	7.099634585	15.88797092
75	3.975	1	3.51758	95.834	-577.520234755	6.011596461	2.466773336	7.755131773	16.23350157
76	3.950	1	3.47269	96.084	-577.520106013	6.334743515	1.876610728	8.434022258	16.6453765
77	3.925	1	3.42789	96.333	-577.519973347	6.667739952	1.33376579	9.138508247	17.14001399
78	3.900	1	3.38320	96.580	-577.519836740	7.01062844	0.855065327	9.865250543	17.73094431
79	3.875	1	3.33862	96.826	-577.519696189	7.363416509	0.460084648	10.61668422	18.44018538
80	3.850	1	3.29415	97.070	-577.519551711	7.726061491	0.171882716	11.38925088	19.28719509
81	3.825	1	3.24979	97.313	-577.519403331	8.098500632	0.017532073	12.18561574	20.30164844
82	3.800	1	3.20557	97.553	-577.519251066	8.480691264	0.028651691	12.99856174	21.5079047
83	3.800	2	3.20782	97.484	-577.519231932	8.528718292	0.023532768	12.76215132	21.31440238

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
84	3.825	2	3.25199	97.250	-577.519384425	8.145955373	0.021572021	11.97656691	20.14409431
85	3.850	2	3.29632	97.008	-577.519533009	7.773004184	0.183089936	11.19037186	19.14646598
86	3.875	2	3.34075	96.764	-577.519677683	7.409867235	0.476745097	10.42469914	18.31131147
87	3.900	2	3.38530	96.520	-577.519818424	7.056602259	0.875875063	9.686157433	17.61863475
88	3.925	2	3.42995	96.273	-577.519955216	6.713249414	1.357485112	8.966168725	17.03690325
89	3.950	2	3.47472	96.025	-577.520088061	6.379803682	1.902416381	8.271236419	16.55345648
90	3.975	2	3.51957	95.776	-577.520216978	6.056217371	2.493773005	7.601699561	16.15168994
91	4.000	2	3.56451	95.526	-577.520342006	5.74239259	3.1178447	6.957898566	15.81813586
92	4.025	2	3.60953	95.274	-577.520463202	5.438186267	3.762923653	6.337771584	15.5388815
93	4.050	2	3.65464	95.021	-577.520580636	5.143422699	4.419536557	5.744295525	15.30725478
94	4.075	2	3.69981	94.768	-577.520694389	4.857898574	5.079308772	5.179988857	15.1171962
95	4.100	2	3.74505	94.512	-577.520804548	4.581395518	5.735895006	4.638681071	14.9559716
96	4.125	2	3.79036	94.256	-577.520911201	4.313692649	6.384043137	4.127238543	14.82497433
97	4.150	2	3.83572	93.999	-577.521014431	4.054581632	7.019278475	3.643838669	14.71769878
98	4.175	2	3.88113	93.741	-577.521114316	3.803866687	7.63832196	3.1888328	14.63102145
99	4.200	2	3.92659	93.481	-577.521210927	3.561369599	8.238657711	2.760987107	14.56101442
100	4.225	2	3.97209	93.220	-577.521304325	3.326937256	8.818286897	2.362479646	14.5077038
101	4.250	2	4.01763	92.958	-577.521394557	3.100451688	9.375888696	1.993667234	14.47000762
102	4.275	2	4.06321	92.695	-577.521481653	2.881837592	9.91059166	1.65490806	14.44733731
103	4.300	2	4.10881	92.431	-577.521565628	2.67105732	10.42167753	1.346561675	14.43929652
104	4.325	2	4.15444	92.165	-577.521646490	2.468090788	10.90908877	1.068002166	14.44518173
105	4.350	2	4.20008	91.898	-577.521724240	2.272935489	11.37269934	0.820821547	14.46645637
106	4.375	2	4.24575	91.630	-577.521798888	2.085566322	11.81300072	0.60538484	14.50395188
107	4.400	2	4.29144	91.361	-577.521870446	1.905953166	12.23033669	0.422058433	14.55834829
108	4.425	2	4.33714	91.090	-577.521938935	1.73404331	12.6251961	0.270713135	14.62995254
109	4.450	2	4.38286	90.818	-577.522004379	1.569776514	12.99834077	0.152462466	14.72057975
110	4.475	2	4.42861	90.545	-577.522066806	1.413082497	13.35058452	0.067678284	14.8313453
111	4.500	2	4.47438	90.270	-577.522126245	1.263888467	13.68263361	0.016610544	14.96313262
112	4.525	2	4.52018	89.994	-577.522182727	1.122116614	13.9953782	8.20274E-06	15.11750302
113	4.550	2	4.56602	89.717	-577.522236283	0.987689126	14.28971224	0.018248585	15.29564995
114	4.575	2	4.61190	89.438	-577.522286939	0.860540742	14.56646534	0.071966265	15.49897235
115	4.600	2	4.65782	89.158	-577.522334718	0.740613732	14.82646816	0.161540162	15.72862205
116	4.625	2	4.70379	88.876	-577.522379639	0.627860405	15.07059612	0.28786506	15.98632158
117	4.650	2	4.74981	88.593	-577.522421717	0.52224311	15.2996508	0.451070606	16.27296452
118	4.675	2	4.79588	88.308	-577.522460958	0.423746788	15.51441723	0.652314526	16.59047854
119	4.700	2	4.84201	88.022	-577.522497367	0.332358887	15.71570223	0.891474462	16.93953558
120	4.725	2	4.88820	87.734	-577.522530941	0.248086938	15.90423893	1.169973818	17.32229969
121	4.750	2	4.93444	87.445	-577.522561674	0.170946002	16.08069899	1.487435495	17.73908049
122	4.775	2	4.98074	87.154	-577.522589557	0.100958668	16.24580653	1.845551308	18.19231651
123	4.800	2	5.02709	86.862	-577.522614581	0.038147527	16.40018406	2.243686684	18.68201827
124	4.800	3	5.02853	86.817	-577.522595688	0.085569637	16.40481277	2.308498567	18.79888097
125	4.775	3	4.98214	87.108	-577.522570380	0.149093628	16.25062592	1.905692871	18.30541242
126	4.750	3	4.93590	87.398	-577.522542194	0.219841503	16.08607862	1.542662479	17.8485826

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
127	4.725	3	4.88969	87.687	-577.522511151	0.297760551	15.91011264	1.219010924	17.42688411
128	4.700	3	4.84354	87.974	-577.522477262	0.38282316	15.72215154	0.935266145	17.04024085
129	4.675	3	4.79744	88.259	-577.522440531	0.475019293	15.52144464	0.690643413	16.68710735
130	4.650	3	4.75139	88.543	-577.522400960	0.574343927	15.30725251	0.483699274	16.36529572
131	4.625	3	4.70540	88.825	-577.522358546	0.680804594	15.0788637	0.314580693	16.07424898
132	4.600	3	4.65947	89.106	-577.522313282	0.794418864	14.83550521	0.182108983	15.81203306
133	4.575	3	4.61359	89.385	-577.522265154	0.915221876	14.57633021	0.086180015	15.5777321
134	4.550	3	4.56775	89.662	-577.522214145	1.043256303	14.30046604	0.026030933	15.36975327
135	4.525	3	4.52195	89.939	-577.522160230	1.178584894	14.0070845	0.000847844	15.18651724
136	4.500	3	4.47619	90.213	-577.522103386	1.32126538	13.69535812	0.0103375	15.026961
137	4.475	3	4.43047	90.486	-577.522043583	1.471373063	13.36446941	0.053818163	14.88966064
138	4.450	3	4.38477	90.758	-577.521980792	1.628980733	13.01346405	0.130916608	14.77336139
139	4.425	3	4.33911	91.028	-577.521914985	1.794158673	12.64172033	0.240792281	14.67667129
140	4.400	3	4.29347	91.297	-577.521846134	1.966977161	12.24835057	0.383297763	14.59862549
141	4.375	3	4.24784	91.565	-577.521774218	2.14748891	11.83259231	0.558065296	14.53814651
142	4.350	3	4.20225	91.831	-577.521699217	2.33574412	11.39415146	0.763893862	14.49378944
143	4.325	3	4.15667	92.096	-577.521621118	2.531775422	10.9322948	1.001011089	14.46508131
144	4.300	3	4.11112	92.360	-577.521539916	2.735595365	10.44692965	1.269054689	14.4515797
145	4.275	3	4.06559	92.623	-577.521455606	2.9472165	9.937859163	1.56766374	14.4527394
146	4.250	3	4.02010	92.884	-577.521368182	3.166653888	9.405469569	1.895164201	14.46728766
147	4.225	3	3.97464	93.144	-577.521277631	3.393940157	8.850115001	2.252274951	14.49633011
148	4.200	3	3.92921	93.403	-577.521183921	3.629155631	8.27262501	2.638640538	14.54042118
149	4.175	3	3.88383	93.660	-577.521087005	3.87241828	7.674540234	3.052238758	14.59919727
150	4.150	3	3.83849	93.917	-577.520986823	4.123878706	7.057552452	3.495936014	14.67736717
151	4.125	3	3.79319	94.172	-577.520883302	4.383720143	6.424111885	3.965928969	14.773761
152	4.100	3	3.74796	94.427	-577.520776365	4.652135863	5.777855527	4.465554314	14.8955457
153	4.075	3	3.70279	94.680	-577.520665923	4.929349259	5.122751637	4.990545715	15.04264661
154	4.050	3	3.65768	94.932	-577.520551888	5.215581214	4.463948273	5.542458729	15.22198822
155	4.025	3	3.61264	95.183	-577.520434167	5.511065162	3.807963336	6.120948842	15.43997734
156	4.000	3	3.56767	95.433	-577.520312683	5.815994375	3.162597253	6.725672905	15.70426453
157	3.975	3	3.52279	95.682	-577.520187361	6.130557107	2.537590707	7.356289139	16.02443695
158	3.950	3	3.47799	95.929	-577.520058144	6.454896429	1.944179497	8.00975501	16.40883094
159	3.925	3	3.43330	96.175	-577.519924993	6.789110232	1.396336654	8.688208927	16.87365581
160	3.900	3	3.38871	96.420	-577.519787889	7.133246208	0.910048598	9.391314577	17.43460938
161	3.875	3	3.34422	96.662	-577.519646830	7.487309376	0.504397014	10.11266426	18.10437065
162	3.850	3	3.29986	96.903	-577.519501834	7.851254556	0.202044509	10.85755602	18.91085509
163	3.825	3	3.25562	97.142	-577.519352925	8.225021507	0.029115442	11.6224055	19.87654245
164	3.800	3	3.21151	97.379	-577.519200125	8.608555008	0.016258414	12.40655922	21.03137264
165	3.800	4	3.21670	97.230	-577.519155432	8.720736046	0.008343176	11.91058044	20.63965967
166	3.825	4	3.26067	96.997	-577.519308723	8.335970118	0.0413955	11.15526983	19.53263545
167	3.850	4	3.30483	96.759	-577.519458092	7.961048551	0.230036099	10.4092928	18.60037745
168	3.875	4	3.34910	96.521	-577.519603547	7.595951264	0.544334606	9.689128875	17.82941475
169	3.900	4	3.39350	96.281	-577.519745055	7.24076109	0.958835222	8.989052541	17.18864885

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)^3**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
170	3.925	4	3.43801	96.039	-577.519882602	6.895513168	1.451531942	8.309720019	16.65676513
171	3.950	4	3.48263	95.796	-577.520016187	6.560210009	2.003841135	7.654434052	16.2184852
172	3.975	4	3.52733	95.551	-577.520145834	6.234791372	2.599635499	7.020996988	15.85542386
173	4.000	4	3.57212	95.305	-577.520271582	5.919159365	3.225776984	6.412496019	15.55743237
174	4.025	4	3.61699	95.057	-577.520393488	5.613170917	3.871036167	5.826962717	15.3111698
175	4.050	4	3.66193	94.809	-577.520511626	5.316640283	4.526049335	5.269457258	15.11214688
176	4.075	4	3.70694	94.559	-577.520626079	5.029359133	5.183216626	4.73582359	14.94839935
177	4.100	4	3.75201	94.309	-577.520736940	4.751094032	5.836186334	4.23067165	14.81795202
178	4.125	4	3.79714	94.057	-577.520844301	4.481614057	6.479947332	3.750302915	14.7118643
179	4.150	4	3.84233	93.804	-577.520948250	4.220698325	7.110505369	3.2971397	14.62834339
180	4.175	4	3.88756	93.550	-577.521048869	3.968141013	7.724461417	2.871527886	14.56413032
181	4.200	4	3.93284	93.295	-577.521146230	3.723761398	8.319569391	2.473814723	14.51714551
182	4.225	4	3.97816	93.039	-577.521240394	3.487406368	8.893933601	2.104348827	14.4856888
183	4.250	4	4.02352	92.782	-577.521331407	3.258960461	9.446313938	1.763480182	14.46875458
184	4.275	4	4.06892	92.523	-577.521419299	3.038348377	9.97590149	1.450410159	14.46466003
185	4.300	4	4.11435	92.263	-577.521504085	2.825532465	10.48213559	1.166877968	14.47454602
186	4.325	4	4.15981	92.001	-577.521585771	2.620497664	10.96487377	0.912326961	14.49769839
187	4.350	4	4.20530	91.739	-577.521664358	2.423241465	11.42421293	0.689057551	14.53651195
188	4.375	4	4.25081	91.475	-577.521739854	2.233743787	11.86034969	0.495724488	14.58981796
189	4.400	4	4.29635	91.209	-577.521812269	2.05197953	12.27383088	0.333049613	14.65886002
190	4.425	4	4.34191	90.942	-577.521881621	1.877903514	12.66513671	0.202189286	14.74522951
191	4.450	4	4.38750	90.674	-577.521947931	1.711463027	13.03501613	0.103508526	14.84998769
192	4.475	4	4.43313	90.404	-577.522011223	1.552597828	13.38426799	0.037189391	14.97405521
193	4.500	4	4.47879	90.133	-577.522071527	1.401232617	13.71358316	0.004030506	15.11884628
194	4.525	4	4.52448	89.861	-577.522128868	1.257304643	14.02376895	0.004402364	15.28547595
195	4.550	4	4.57022	89.586	-577.522183274	1.120743624	14.31577584	0.039053235	15.4755727
196	4.575	4	4.61601	89.310	-577.522234768	0.99149183	14.59041622	0.108481208	15.69038926
197	4.600	4	4.66184	89.033	-577.522283373	0.86949153	14.84844934	0.21306361	15.93100448
198	4.625	4	4.70773	88.754	-577.522329105	0.754702564	15.09079539	0.353746716	16.19924467
199	4.650	4	4.75367	88.473	-577.522371978	0.647089791	15.31819199	0.531293382	16.49657516
200	4.675	4	4.79967	88.191	-577.522411999	0.54663564	15.53146296	0.745647328	16.82374592
201	4.700	4	4.84572	87.907	-577.522449172	0.453330072	15.73131615	0.99814765	17.18279387
202	4.725	4	4.89184	87.621	-577.522483495	0.367178106	15.91856569	1.289570875	17.57531467
203	4.750	4	4.93801	87.334	-577.522514962	0.288194804	16.09383297	1.619483853	18.00151163
204	4.775	4	4.98424	87.045	-577.522543567	0.216395224	16.25783637	1.989625335	18.46385693
205	4.800	4	5.03052	86.755	-577.522569299	0.151806977	16.41119315	2.399306521	18.96230664
206	4.800	5	5.03306	86.676	-577.522535315	0.237108041	16.41930965	2.517551493	19.17396918
207	4.775	5	4.98684	86.961	-577.522509069	0.302986446	16.26673271	2.104348827	18.67406799
208	4.750	5	4.94069	87.250	-577.522479940	0.376101284	16.10364759	1.723144585	18.20289345
209	4.725	5	4.89458	87.535	-577.522447934	0.456437497	15.92930011	1.384491135	17.77022874
210	4.700	5	4.84853	87.819	-577.522413066	0.543957432	15.74308667	1.08384621	17.37089032
211	4.675	5	4.80253	88.102	-577.522375338	0.63865607	15.54426471	0.820821547	17.00374232
212	4.650	5	4.75659	88.382	-577.522334751	0.740530901	15.33215044	0.596504009	16.66918535

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
213	4.625	5	4.71071	88.661	-577.522291302	0.849589455	15.10599863	0.408523916	16.364112
214	4.600	5	4.66488	88.938	-577.522244984	0.965849302	14.86499019	0.256983574	16.08782307
215	4.575	5	4.61911	89.213	-577.522195783	1.089345584	14.60839166	0.141125599	15.83886284
216	4.550	5	4.57340	89.487	-577.522143683	1.22011846	14.33541064	0.059964064	15.61549317
217	4.525	5	4.52772	89.759	-577.522088663	1.35822064	14.04505282	0.013233978	15.41650744
218	4.500	5	4.48210	90.030	-577.522030699	1.503712367	13.73669437	0.000205068	15.24061181
219	4.475	5	4.43652	90.298	-577.521969765	1.656658901	13.4094008	0.020234331	15.08629403
220	4.450	5	4.39097	90.566	-577.521905837	1.817120482	13.06230188	0.072994341	14.9524167
221	4.425	5	4.34547	90.831	-577.521838890	1.985159862	12.69479081	0.157346968	14.83729765
222	4.400	5	4.30000	91.096	-577.521768898	2.160842302	12.30599523	0.273701666	14.7405392
223	4.375	5	4.25456	91.358	-577.521695842	2.344215492	11.8952574	0.42019983	14.65967272
224	4.350	5	4.20915	91.619	-577.521619708	2.535314573	11.46200919	0.597241572	14.59456534
225	4.325	5	4.16378	91.879	-577.521540484	2.734169665	11.00590246	0.804470072	14.5445422
226	4.300	5	4.11844	92.137	-577.521458167	2.940788298	10.52654243	1.040555805	14.50788654
227	4.275	5	4.07312	92.394	-577.521372755	3.155175493	10.02370094	1.30588407	14.4847605
228	4.250	5	4.02785	92.650	-577.521284242	3.377346309	9.497836389	1.600103518	14.47528622
229	4.225	5	3.98262	92.904	-577.521192616	3.607330868	8.949258788	1.92154056	14.47813022
230	4.200	5	3.93742	93.157	-577.521097847	3.84520447	8.378604226	2.270939142	14.49474784
231	4.175	5	3.89227	93.409	-577.520999889	4.091082576	7.787308581	2.647953379	14.52634454
232	4.150	5	3.84719	93.660	-577.520898683	4.345113279	7.177345653	3.052238758	14.57469769
233	4.125	5	3.80211	93.910	-577.520794156	4.607479813	6.550047283	3.48345213	14.64097923
234	4.100	5	3.75710	94.158	-577.520686223	4.878395528	5.909379384	3.939356655	14.72713157
235	4.075	5	3.71216	94.406	-577.520574797	5.158078799	5.259208533	4.423289024	14.84057636
236	4.050	5	3.66727	94.652	-577.520459780	5.44677561	4.604089665	4.931008421	14.9818737
237	4.025	5	3.62245	94.897	-577.520341079	5.744719393	3.950316812	5.464073594	15.1591098
238	4.000	5	3.57771	95.141	-577.520218608	6.052126012	3.305389783	6.022149599	15.37966539
239	3.975	5	3.53304	95.384	-577.520092293	6.36918121	2.67809119	6.604902856	15.65217526
240	3.950	5	3.48847	95.625	-577.519962075	6.696033077	2.079578645	7.209437573	15.9850493
241	3.925	5	3.44399	95.865	-577.519827914	7.032782017	1.522542118	7.837767294	16.39309143
242	3.900	5	3.39962	96.103	-577.519689789	7.37948074	1.022461839	8.486782496	16.88872507
243	3.875	5	3.35536	96.340	-577.519547699	7.736131755	0.597314482	9.158721388	17.49216763
244	3.850	5	3.31123	96.574	-577.519401661	8.102692392	0.268396	9.847267407	18.2183558
245	3.825	5	3.26723	96.806	-577.519251705	8.479087351	0.060374079	10.55456215	19.09402358
246	3.800	5	3.22337	97.036	-577.519097854	8.865258899	0.002051476	11.27997127	20.14728165
247	3.800	6	3.23150	96.805	-577.519027191	9.042625573	0.000103667	10.55146083	19.59419007
248	3.825	6	3.27513	96.581	-577.519181774	8.654616678	0.087626009	9.868249327	18.61049201
249	3.850	6	3.31897	96.352	-577.519332450	8.276414494	0.318154612	9.193424438	17.78799354
250	3.875	6	3.36293	96.123	-577.519479208	7.908046631	0.663916092	8.542497314	17.11446004
251	3.900	6	3.40704	95.891	-577.519622019	7.549585879	1.101479456	7.907412184	16.55847752
252	3.925	6	3.45126	95.657	-577.519760863	7.201082441	1.610218935	7.291698274	16.10299965
253	3.950	6	3.49558	95.421	-577.519895744	6.862526275	2.172714669	6.6959954	15.73123634
254	3.975	6	3.54000	95.184	-577.520026681	6.533869692	2.774322713	6.123311002	15.43150341
255	4.000	6	3.58450	94.945	-577.520153715	6.215009778	3.402437718	5.571715389	15.18916289

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
256	4.025	6	3.62908	94.705	-577.520276907	5.905793423	4.046735769	5.04400592	14.99653511
257	4.050	6	3.67374	94.464	-577.520396330	5.606037394	4.698647133	4.540510705	14.84519523
258	4.075	6	3.71846	94.222	-577.520512072	5.315520808	5.350818327	4.061559221	14.72789836
259	4.100	6	3.76324	93.979	-577.520624225	5.03401274	5.997490154	3.607482312	14.63898521
260	4.125	6	3.80809	93.734	-577.520732893	4.761252148	6.634159753	3.176910348	14.57232225
261	4.150	6	3.85299	93.488	-577.520838164	4.497018148	7.256849009	2.7721025	14.52596966
262	4.175	6	3.89794	93.242	-577.520940123	4.241097388	7.862681089	2.394872257	14.49865073
263	4.200	6	3.94293	92.993	-577.521038842	3.993309144	8.449335878	2.041125769	14.48377079
264	4.225	6	3.98798	92.744	-577.521134379	3.753507834	9.015458752	1.715633612	14.4846002
265	4.250	6	4.03308	92.493	-577.521226778	3.521583018	9.559784396	1.416122715	14.49749013
266	4.275	6	4.07821	92.241	-577.521316066	3.297466924	10.08135717	1.144300388	14.52312448
267	4.300	6	4.12339	91.987	-577.521402256	3.081126921	10.58002842	0.899605426	14.56076076
268	4.325	6	4.16861	91.732	-577.521485352	2.872552969	11.05557541	0.683521386	14.61164976
269	4.350	6	4.21387	91.476	-577.521565354	2.671745069	11.50811809	0.496396884	14.67626004
270	4.375	6	4.25917	91.218	-577.521642266	2.478693181	11.93795774	0.338026625	14.75467754
271	4.400	6	4.30450	90.958	-577.521716095	2.293379733	12.3454528	0.209116042	14.84794857
272	4.425	6	4.34987	90.697	-577.521786857	2.115764565	12.73125967	0.110693441	14.95771768
273	4.450	6	4.39528	90.434	-577.521854569	1.945805008	13.09602453	0.042917636	15.08474717
274	4.475	6	4.44073	90.170	-577.521919255	1.783440819	13.44045863	0.006584976	15.23048442
275	4.500	6	4.48622	89.904	-577.521980937	1.628616778	13.7653198	0.002099901	15.39603648
276	4.525	6	4.53176	89.636	-577.522039641	1.481267625	14.07146221	0.030189721	15.58291955
277	4.550	6	4.57735	89.366	-577.522095392	1.341330608	14.35968138	0.091587214	15.7925992
278	4.575	6	4.62299	89.095	-577.522148212	1.208750506	14.6307817	0.186617983	16.02615018
279	4.600	6	4.66868	88.822	-577.522198122	1.08347461	14.88556769	0.316189114	16.28523141
280	4.625	6	4.71442	88.548	-577.522245139	0.965460247	15.12483699	0.48038514	16.57068238
281	4.650	6	4.76022	88.271	-577.522289277	0.854672278	15.34942213	0.68115558	16.88524999
282	4.675	6	4.80609	87.993	-577.522330545	0.751088112	15.56012645	0.91780639	17.22902095
283	4.700	6	4.85201	87.713	-577.522368944	0.65470524	15.75759751	1.191759606	17.60406235
284	4.725	6	4.89798	87.432	-577.522404480	0.565508601	15.94256074	1.502610332	18.01067968
285	4.750	6	4.94401	87.149	-577.522437146	0.483515765	16.11575262	1.852041725	18.4513101
286	4.775	6	4.99010	86.864	-577.522466936	0.408741792	16.27783926	2.240827575	18.92740863
287	4.800	6	5.03625	86.577	-577.522493843	0.341204254	16.42946	2.669747142	19.44041139
288	4.800	7	5.03982	86.464	-577.522445221	0.463247224	16.44076267	2.848923875	19.75293377
289	4.775	7	4.99393	86.741	-577.522416969	0.534160761	16.29081968	2.420053979	19.24503442
290	4.750	7	4.94791	87.027	-577.522386431	0.610812241	16.12989727	2.01393825	18.75464776
291	4.725	7	4.90199	87.307	-577.522353001	0.694722744	15.95811624	1.652452707	18.30529169
292	4.700	7	4.85611	87.586	-577.522316690	0.785864661	15.77460004	1.327794494	17.88825919
293	4.675	7	4.81029	87.863	-577.522277503	0.884225442	15.57873569	1.040555805	17.50351694
294	4.650	7	4.76452	88.139	-577.522235441	0.989802576	15.36976641	0.789130953	17.14869994
295	4.625	7	4.71882	88.412	-577.522190498	1.102611124	15.14705139	0.574589027	16.82425154
296	4.600	7	4.67318	88.684	-577.522142662	1.222681206	14.90979475	0.394610022	16.52708598
297	4.575	7	4.62759	88.953	-577.522091927	1.350027883	14.65717135	0.249775419	16.25697465
298	4.550	7	4.58205	89.221	-577.522038272	1.484703864	14.3883903	0.138271046	16.01136521

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
299	4.525	7	4.53656	89.488	-577.521981676	1.626761862	14.10265325	0.059730514	15.78914563
300	4.500	7	4.49112	89.752	-577.521922117	1.776257096	13.79916126	0.014013922	15.58943228
301	4.475	7	4.44573	90.015	-577.521859569	1.933254828	13.47712318	5.12671E-05	15.41042928
302	4.450	7	4.40039	90.276	-577.521794009	2.097812788	13.13576589	0.017356993	15.25093567
303	4.425	7	4.35509	90.536	-577.521725411	2.269996237	12.77426452	0.065461494	15.10972225
304	4.400	7	4.30983	90.794	-577.521653755	2.449855377	12.39190733	0.143647257	14.98540997
305	4.375	7	4.26461	91.050	-577.521579023	2.637435387	11.98804477	0.251208847	14.876689
306	4.350	7	4.21944	91.304	-577.521501201	2.832771409	11.56220759	0.387446297	14.7824253
307	4.325	7	4.17431	91.557	-577.521420284	3.035875992	11.11385213	0.552374418	14.70210254
308	4.300	7	4.12922	91.809	-577.521336266	3.246764196	10.64266044	0.745647328	14.63507197
309	4.275	7	4.08418	92.059	-577.521249146	3.465438533	10.14860113	0.965981981	14.58002164
310	4.250	7	4.03919	92.307	-577.521158928	3.691888961	9.631761952	1.212694816	14.53634573
311	4.225	7	3.99426	92.554	-577.521065599	3.92614811	9.092617506	1.48627139	14.50503701
312	4.200	7	3.94937	92.799	-577.520969133	4.168281243	8.531600603	1.78509827	14.48498012
313	4.175	7	3.90454	93.043	-577.520869489	4.41839127	7.950020493	2.109892055	14.47830382
314	4.150	7	3.85977	93.286	-577.520766610	4.676621264	7.349413487	2.460319169	14.48635392
315	4.125	7	3.81505	93.527	-577.520660428	4.943141907	6.731726222	2.83443989	14.50930802
316	4.100	7	3.77039	93.767	-577.520550857	5.218169061	6.09983182	3.23331169	14.55131257
317	4.075	7	3.72579	94.006	-577.520437805	5.501933651	5.457243426	3.656606458	14.61578354
318	4.050	7	3.68126	94.244	-577.520321174	5.79468166	4.808529743	4.103997452	14.70720885
319	4.025	7	3.63680	94.480	-577.520200867	6.096656561	4.159180678	4.573117499	14.82895474
320	4.000	7	3.59242	94.715	-577.520076796	6.408079237	3.516071538	5.06546975	14.98962053
321	3.975	7	3.54811	94.949	-577.519948886	6.729137942	2.887231593	5.580732932	15.19710247
322	3.950	7	3.50390	95.181	-577.519817077	7.059983277	2.282923019	6.116225888	15.45913218
323	3.925	7	3.45978	95.411	-577.519681329	7.400715644	1.714761507	6.671314273	15.78679142
324	3.900	7	3.41578	95.639	-577.519541621	7.751387754	1.197072247	7.245369211	16.19382921
325	3.875	7	3.37190	95.865	-577.519397951	8.112004626	0.746275952	7.837767294	16.69604787
326	3.850	7	3.32814	96.089	-577.519250338	8.48251857	0.381685615	8.447890581	17.31209477
327	3.825	7	3.28452	96.311	-577.519098811	8.862856795	0.126024595	9.075126603	18.06400799
328	3.800	7	3.24105	96.529	-577.518943397	9.25295153	0.005541651	9.712916814	18.97140999
329	3.800	8	3.25208	96.219	-577.518846328	9.496598214	0.021745886	8.812465823	18.33080992
330	3.825	8	3.29523	96.008	-577.519002722	9.104043644	0.177421066	8.224626412	17.50609112
331	3.850	8	3.33857	95.794	-577.519155240	8.721217973	0.45969645	7.6491524	16.83006682
332	3.875	8	3.38207	95.576	-577.519303852	8.348196503	0.843942992	7.084380227	16.27651972
333	3.900	8	3.42572	95.357	-577.519448528	7.985054535	1.30892351	6.538823651	15.8328017
334	3.925	8	3.46949	95.134	-577.519589252	7.631832229	1.836123647	6.005761212	15.47371709
335	3.950	8	3.51337	94.910	-577.519726023	7.288532095	2.40986121	5.493122906	15.19151621
336	3.975	8	3.55735	94.684	-577.519858858	6.955111463	3.01680913	4.999080208	14.9710008
337	4.000	8	3.60143	94.456	-577.519987807	6.631444831	3.645850664	4.524251056	14.80154655
338	4.025	8	3.64559	94.227	-577.520112925	6.317394147	4.28739073	4.071184906	14.67596978
339	4.050	8	3.68983	93.996	-577.520234287	6.012771158	4.933692137	3.638373595	14.58483689
340	4.075	8	3.73414	93.764	-577.520351981	5.717354981	5.578238608	3.228163789	14.52375738
341	4.100	8	3.77853	93.530	-577.520466102	5.430907162	6.215979783	2.839263784	14.48615073

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
342	4.125	8	3.82298	93.295	-577.520576749	5.153179209	6.842443034	2.473814723	14.46943697
343	4.150	8	3.86750	93.058	-577.520684015	4.883937687	7.454448456	2.130744098	14.46913024
344	4.175	8	3.91209	92.820	-577.520787977	4.622989325	8.049402502	1.811984794	14.48437662
345	4.200	8	3.95673	92.581	-577.520888711	4.370143358	8.62507807	1.517862184	14.51308361
346	4.225	8	4.00144	92.340	-577.520986268	4.125271776	9.180297401	1.247636429	14.55320561
347	4.250	8	4.04621	92.097	-577.521080685	3.888281707	9.713934303	1.00196648	14.60418249
348	4.275	8	4.09104	91.853	-577.521171984	3.659117931	10.22536234	0.78236096	14.66684123
349	4.300	8	4.13593	91.607	-577.521260175	3.437755346	10.71426119	0.588420894	14.74043743
350	4.325	8	4.18087	91.360	-577.521345256	3.224198973	11.18046191	0.421438443	14.82609933
351	4.350	8	4.22586	91.111	-577.521427230	3.018441282	11.6241187	0.281244767	14.92380475
352	4.375	8	4.27090	90.860	-577.521506095	2.820487293	12.04555264	0.168520692	15.03456062
353	4.400	8	4.31599	90.607	-577.521581860	2.630314415	12.44521797	0.083952516	15.1594849
354	4.425	8	4.36112	90.353	-577.521654536	2.447895039	12.82359206	0.028392638	15.29987973
355	4.450	8	4.40631	90.097	-577.521724142	2.273181473	13.18148163	0.002143877	15.45680698
356	4.475	8	4.45153	89.840	-577.521790697	2.106126027	13.51935453	0.005833058	15.63131361
357	4.500	8	4.49681	89.581	-577.521854226	1.94666595	13.83818291	0.040002246	15.8248511
358	4.525	8	4.54213	89.320	-577.521914754	1.794738491	14.13859533	0.105359611	16.03869343
359	4.550	8	4.58750	89.057	-577.521972306	1.650280899	14.42145004	0.20261879	16.27434973
360	4.575	8	4.63293	88.792	-577.522026905	1.513235444	14.68759617	0.332498891	16.5333305
361	4.600	8	4.67841	88.526	-577.522078574	1.383544393	14.93776085	0.495052547	16.81635779
362	4.625	8	4.72394	88.258	-577.522127330	1.261165078	15.17272749	0.691437028	17.12532959
363	4.650	8	4.76953	87.988	-577.522173190	1.146054827	15.39331299	0.922385113	17.46175293
364	4.675	8	4.81517	87.716	-577.522216164	1.03818854	15.60021714	1.188635047	17.82704073
365	4.700	8	4.86088	87.442	-577.522256259	0.937548647	15.79425433	1.490930545	18.22273352
366	4.725	8	4.90664	87.166	-577.522293477	0.844130127	15.97604083	1.830020791	18.65019175
367	4.750	8	4.95246	86.889	-577.522327816	0.757938001	16.14629734	2.205242503	19.10947785
368	4.775	8	4.99834	86.610	-577.522359271	0.678984818	16.30567517	2.618518994	19.60317898
369	4.800	8	5.04427	86.329	-577.522387836	0.60728564	16.45476785	3.070613119	20.13266661
370	4.800	9	5.04892	86.181	-577.522323851	0.767890293	16.46930395	3.323193646	20.56038789
371	4.775	9	5.00327	86.453	-577.522293502	0.844067376	16.32216817	2.86667665	20.0329122
372	4.750	9	4.95758	86.730	-577.522261062	0.925492944	16.16462135	2.436418213	19.5265325
373	4.725	9	4.91191	87.004	-577.522225707	1.014235267	15.99620882	2.045219619	19.05566371
374	4.700	9	4.86628	87.276	-577.522187466	1.110221553	15.81634103	1.690715517	18.6172781
375	4.675	9	4.82071	87.546	-577.522146344	1.213439254	15.62442167	1.372162192	18.21002312
376	4.650	9	4.77520	87.814	-577.522102337	1.323898408	15.4197591	1.088821398	17.8324789
377	4.625	9	4.72975	88.080	-577.522055438	1.441616586	15.20163936	0.839960357	17.4832163
378	4.600	9	4.68435	88.345	-577.522005633	1.566628929	14.96927583	0.624097335	17.16000209
379	4.575	9	4.63901	88.607	-577.521952903	1.698983127	14.72196395	0.442138736	16.86308581
380	4.550	9	4.59372	88.868	-577.521897236	1.838709302	14.4588801	0.291977366	16.58956677
381	4.525	9	4.54849	89.126	-577.521838606	1.985872712	14.17930531	0.174052072	16.3392301
382	4.500	9	4.50330	89.383	-577.521776989	2.1405336	13.882331	0.086741446	16.10960605
383	4.475	9	4.45817	89.638	-577.521712359	2.302757227	13.56730927	0.029858877	15.89992538
384	4.450	9	4.41308	89.891	-577.521644691	2.472606343	13.23333571	0.002707131	15.70864919

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
385	4.425	9	4.36804	90.143	-577.521573961	2.65014119	12.87973932	0.004659383	15.53453989
386	4.400	9	4.32304	90.393	-577.521500147	2.835416987	12.50573581	0.035191796	15.37634459
387	4.375	9	4.27809	90.641	-577.521423231	3.028478916	12.11075855	0.093620809	15.23285828
388	4.350	9	4.23320	90.888	-577.521343202	3.229354587	11.69433583	0.17967277	15.10336319
389	4.325	9	4.18836	91.132	-577.521260046	3.438079141	11.2559147	0.291977366	14.9859712
390	4.300	9	4.14358	91.375	-577.521173772	3.654629986	10.79525953	0.430786146	14.88067566
391	4.275	9	4.09885	91.617	-577.521084377	3.879014655	10.31209278	0.595766902	14.78687434
392	4.250	9	4.05419	91.857	-577.520991862	4.111230635	9.806659944	0.78574231	14.70363289
393	4.225	9	4.00960	92.095	-577.520896218	4.351300518	9.279245994	1.000056154	14.63060267
394	4.200	9	3.96508	92.331	-577.520797427	4.599269485	8.73042647	1.238057682	14.56775364
395	4.175	9	3.92062	92.566	-577.520695452	4.855230406	8.160995729	1.500270729	14.51649686
396	4.150	9	3.87625	92.798	-577.520590244	5.119306273	7.572686986	1.783822972	14.47581623
397	4.125	9	3.83194	93.030	-577.520481738	5.39166024	6.966947281	2.091903223	14.45051074
398	4.100	9	3.78772	93.260	-577.520369854	5.672493107	6.346616384	2.421539358	14.44064885
399	4.075	9	3.74356	93.488	-577.520254502	5.96203078	5.714394739	2.7721025	14.44852802
400	4.050	9	3.69949	93.714	-577.520135585	6.260516731	5.074642624	3.142969242	14.4781286
401	4.025	9	3.65550	93.939	-577.520013008	6.568189414	4.432099498	3.535316447	14.53560536
402	4.000	9	3.61160	94.162	-577.519886686	6.885262181	3.792896662	3.946939631	14.62509847
403	3.975	9	3.56779	94.384	-577.519756542	7.211928307	3.164298585	4.37922665	14.75545354
404	3.950	9	3.52407	94.603	-577.519622513	7.548345922	2.555052613	4.827677848	14.93107638
405	3.925	9	3.48047	94.821	-577.519484570	7.894587817	1.976009882	5.295788047	15.16638575
406	3.900	9	3.43697	95.036	-577.519342686	8.250721765	1.439287914	5.778668414	15.46867809
407	3.875	9	3.39360	95.249	-577.519196861	8.616747765	0.959863323	6.277828938	15.85444003
408	3.850	9	3.35036	95.459	-577.519047112	8.992623146	0.554842131	6.790199287	16.33766456
409	3.825	9	3.30727	95.666	-577.518893471	9.378267587	0.244357435	7.314918175	16.9375432
410	3.800	9	3.26432	95.871	-577.518735963	9.773618337	0.05153912	7.853811849	17.67896931
411	3.800	10	3.27806	95.486	-577.518612174	10.08433318	0.098919985	6.857533511	17.04078668
412	3.825	10	3.32058	95.294	-577.518770930	9.685849909	0.328955404	6.385930769	16.40073608
413	3.850	10	3.36333	95.095	-577.518925843	9.297012702	0.667510474	5.914863256	15.87938643
414	3.875	10	3.40624	94.893	-577.519076877	8.917911925	1.092863734	5.455150838	15.4659265
415	3.900	10	3.44930	94.689	-577.519224001	8.548625388	1.586439234	5.009758578	15.1448232
416	3.925	10	3.49249	94.481	-577.519367200	8.189190743	2.132115876	4.575159297	14.89646592
417	3.950	10	3.53581	94.271	-577.519506471	7.839615519	2.716313342	4.156382187	14.71231105
418	3.975	10	3.57924	94.058	-577.519641835	7.499847006	3.327225773	3.752151949	14.57922473
419	4.000	10	3.62278	93.844	-577.519773331	7.169787312	3.955112247	3.366844743	14.4917443
420	4.025	10	3.66641	93.627	-577.519901018	6.849288345	4.591520876	2.99744652	14.43825574
421	4.050	10	3.71014	93.408	-577.520024968	6.538169383	5.229810487	2.6464001	14.41437997
422	4.075	10	3.75396	93.188	-577.520145267	6.236214562	5.864242525	2.315756851	14.41621394
423	4.100	10	3.79786	92.966	-577.520262008	5.94319045	6.49011336	2.004465683	14.43776949
424	4.125	10	3.84185	92.742	-577.520375284	5.658863612	7.103893012	1.7131336	14.47589022
425	4.150	10	3.88593	92.516	-577.520485182	5.383015675	7.70266228	1.442373071	14.52805103
426	4.175	10	3.93009	92.288	-577.520591780	5.115450858	8.284017988	1.192802038	14.59227088
427	4.200	10	3.97434	92.059	-577.520695140	4.856013537	8.846374199	0.965981981	14.66836972

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
428	4.225	10	4.01866	91.828	-577.520795308	4.604588251	9.388232409	0.761392711	14.75421337
429	4.250	10	4.06306	91.595	-577.520892317	4.361092169	9.90887094	0.579665839	14.84962895
430	4.275	10	4.10754	91.360	-577.520986186	4.125477599	10.40776808	0.421438443	14.95468413
431	4.300	10	4.15208	91.123	-577.521076920	3.897731993	10.88446771	0.287353072	15.06955278
432	4.325	10	4.19669	90.885	-577.521164514	3.677867899	11.33907977	0.178460816	15.19540849
433	4.350	10	4.24137	90.645	-577.521248974	3.465870259	11.77178539	0.094792889	15.33244854
434	4.375	10	4.28610	90.403	-577.521330299	3.261741581	12.18273755	0.037005513	15.48148464
435	4.400	10	4.33088	90.160	-577.521408494	3.065469316	12.57241747	0.005833058	15.64371984
436	4.425	10	4.37572	89.915	-577.521483575	2.877013303	12.9414796	0.001646244	15.82013915
437	4.450	10	4.42060	89.668	-577.521555558	2.696333382	13.29040512	0.025114961	16.01185346
438	4.475	10	4.46554	89.419	-577.521624467	2.523369311	13.62004809	0.076914567	16.22033197
439	4.500	10	4.51052	89.168	-577.521690325	2.35806336	13.93099715	0.157725889	16.4467864
440	4.525	10	4.55555	88.916	-577.521753160	2.200345248	14.22408687	0.267741009	16.69217313
441	4.550	10	4.60063	88.662	-577.521812997	2.050152224	14.50008931	0.407913951	16.95815548
442	4.575	10	4.64577	88.406	-577.521869862	1.907419027	14.75983631	0.578939213	17.24619455
443	4.600	10	4.69096	88.148	-577.521923779	1.772085416	15.00403803	0.781516761	17.55764021
444	4.625	10	4.73620	87.888	-577.521974768	1.644101191	15.23345843	1.016352032	17.89391165
445	4.650	10	4.78150	87.626	-577.522022847	1.52342117	15.44889336	1.284155929	18.25647046
446	4.675	10	4.82685	87.362	-577.522068029	1.410012723	15.65102288	1.585644825	18.64668043
447	4.700	10	4.87227	87.096	-577.522110322	1.30385577	15.84063926	1.92154056	19.0660356
448	4.725	10	4.91775	86.829	-577.522149733	1.204932742	16.01837755	2.291125168	19.51443546
449	4.750	10	4.96328	86.559	-577.522186257	1.113256187	16.18485957	2.697898939	19.99601469
450	4.775	10	5.00888	86.287	-577.522219898	1.028816066	16.34079048	3.141276971	20.51088352
451	4.800	10	5.05454	86.013	-577.522250648	0.951632459	16.48673882	3.622002981	21.06037426
452	4.800	11	5.06063	85.831	-577.522171057	1.151408734	16.50546808	3.960227382	21.6171042
453	4.775	11	5.01495	86.097	-577.522138009	1.234360404	16.36076648	3.470990577	21.06611746
454	4.750	11	4.96962	86.364	-577.522103124	1.32192301	16.20717173	3.012340641	20.54143538
455	4.725	11	4.92424	86.630	-577.522065294	1.416877672	16.04279264	2.587713156	20.04738346
456	4.700	11	4.87893	86.894	-577.522024586	1.519056217	15.86740828	2.198159666	19.58462416
457	4.675	11	4.83367	87.155	-577.521980989	1.628486256	15.68029532	1.844254592	19.15303617
458	4.650	11	4.78848	87.415	-577.521934504	1.74516528	15.48086704	1.522570556	18.74860287
459	4.625	11	4.74334	87.672	-577.521885116	1.869130938	15.26834347	1.234872969	18.37234737
460	4.600	11	4.69827	87.927	-577.521832811	2.000418371	15.04210732	0.979162869	18.02168856
461	4.575	11	4.65326	88.181	-577.521777569	2.139077779	14.80138459	0.753913865	17.69437624
462	4.550	11	4.60829	88.432	-577.521719370	2.285159365	14.54531589	0.560206894	17.39068215
463	4.525	11	4.56339	88.681	-577.521658189	2.438725877	14.27331536	0.396411206	17.10845244
464	4.500	11	4.51854	88.928	-577.521594002	2.599837558	13.98450681	0.261845975	16.84619034
465	4.475	11	4.47373	89.173	-577.521526781	2.768564688	13.67805659	0.155835842	16.60245712
466	4.450	11	4.42898	89.416	-577.521456501	2.944970018	13.35334925	0.077710916	16.37603018
467	4.425	11	4.38428	89.658	-577.521383134	3.129123829	13.00958777	0.026650695	16.16536229
468	4.400	11	4.33963	89.898	-577.521306660	3.321076322	12.64607529	0.002370591	15.9695222
469	4.375	11	4.29503	90.136	-577.521227058	3.520880208	12.26216351	0.004214384	15.7872581
470	4.350	11	4.25049	90.373	-577.521144315	3.728568117	11.85736369	0.031701075	15.61763288

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
471	4.325	11	4.20601	90.607	-577.521058422	3.944162639	11.43119575	0.083952516	15.4593109
472	4.300	11	4.16159	90.840	-577.520969375	4.167673814	10.98329186	0.160773662	15.31173933
473	4.275	11	4.11724	91.072	-577.520877178	4.399091604	10.51353354	0.261845975	15.17447112
474	4.250	11	4.07297	91.301	-577.520781832	4.638413496	10.02199731	0.38566562	15.04607642
475	4.225	11	4.02878	91.528	-577.520683331	4.885654552	9.508874695	0.531989475	14.92651872
476	4.200	11	3.98467	91.754	-577.520581659	5.140854932	8.974615196	0.700995952	14.81646608
477	4.175	11	3.94065	91.978	-577.520476786	5.404089938	8.420106243	0.891474462	14.71567064
478	4.150	11	3.89672	92.200	-577.520368665	5.67547754	7.846489764	1.102812535	14.62477984
479	4.125	11	3.85289	92.419	-577.520257238	5.955163321	7.255480732	1.333300582	14.54394464
480	4.100	11	3.80915	92.637	-577.520142430	6.243335535	6.649042211	1.584442896	14.47682064
481	4.075	11	3.76550	92.853	-577.520024158	6.540202512	6.029869983	1.854641081	14.42471358
482	4.050	11	3.72196	93.067	-577.519902330	6.845995178	5.401658228	2.143304541	14.39095795
483	4.025	11	3.67852	93.279	-577.519776859	7.160931905	4.768496999	2.449848146	14.37927705
484	4.000	11	3.63519	93.488	-577.519647654	7.485241107	4.135716723	2.7721025	14.39306033
485	3.975	11	3.59196	93.695	-577.519514658	7.819065854	3.509459644	3.11089403	14.43941953
486	3.950	11	3.54885	93.900	-577.519377807	8.162566791	2.897573428	3.465656746	14.52579697
487	3.925	11	3.50585	94.102	-577.519237064	8.515836788	2.308934796	3.833960588	14.65873217
488	3.900	11	3.46298	94.302	-577.519092411	8.878921025	1.754503575	4.216937304	14.8503619
489	3.875	11	3.42024	94.499	-577.518943847	9.251822014	1.246858093	4.61198959	15.1106697
490	3.850	11	3.37765	94.692	-577.518791389	9.634497082	0.800951618	5.016171068	15.45161977
491	3.825	11	3.33519	94.883	-577.518635068	10.02686842	0.433764938	5.432875848	15.89350921
492	3.800	11	3.29289	95.070	-577.518474908	10.42887579	0.16552066	5.856959901	16.45135635
493	3.800	12	3.30926	94.617	-577.518324007	10.80764273	0.25631528	4.85708922	15.92104723
494	3.825	12	3.35101	94.445	-577.518485712	10.40175736	0.560293701	4.501941659	15.46399272
495	3.850	12	3.39301	94.265	-577.518643600	10.00545279	0.953803149	4.144712425	15.10396837
496	3.875	12	3.43522	94.081	-577.518797639	9.618809357	1.41875699	3.794805502	14.83237185
497	3.900	12	3.47760	93.894	-577.518947799	9.241902351	1.939186132	3.45500139	14.63608987
498	3.925	12	3.52012	93.703	-577.519094063	8.874774446	2.501246121	3.124379331	14.5003999
499	3.950	12	3.56279	93.509	-577.519236428	8.517433171	3.093526371	2.805582659	14.4165422
500	3.975	12	3.60559	93.312	-577.519374914	8.169828325	3.705933128	2.499407037	14.37516849
501	4.000	12	3.64852	93.112	-577.519509557	7.831869548	4.330160761	2.206660437	14.36869075
502	4.025	12	3.69155	92.910	-577.519640412	7.503418787	4.958800613	1.929489013	14.39170841
503	4.050	12	3.73470	92.705	-577.519767549	7.18430034	5.586343396	1.667212167	14.4378559
504	4.075	12	3.77797	92.498	-577.519891046	6.874318424	6.208002128	1.421808807	14.50412936
505	4.100	12	3.82134	92.289	-577.520010991	6.573252156	6.819585578	1.193844924	14.58668266
506	4.125	12	3.86481	92.077	-577.520127469	6.280888183	7.417957885	0.982945243	14.68179131
507	4.150	12	3.90839	91.864	-577.520240562	5.997020682	8.000769737	0.791677219	14.78946764
508	4.175	12	3.95207	91.648	-577.520350339	5.72147646	8.565959676	0.618829127	14.90626526
509	4.200	12	3.99585	91.431	-577.520456859	5.454107425	9.112083538	0.466590186	15.03278115
510	4.225	12	4.03973	91.211	-577.520560166	5.194803136	9.638102861	0.334152426	15.16705842
511	4.250	12	4.08370	90.990	-577.520660289	4.943490802	10.14320977	0.223319538	15.31002011
512	4.275	12	4.12775	90.766	-577.520757244	4.700130261	10.62690511	0.133694602	15.46072998
513	4.300	12	4.17188	90.541	-577.520851035	4.464711475	11.08905329	0.066688487	15.62045325

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
514	4.325	12	4.21608	90.314	-577.520941655	4.237252012	11.52962089	0.022465476	15.78933838
515	4.350	12	4.26036	90.085	-577.521029116	4.017721754	11.94894211	0.001646244	15.96831011
516	4.375	12	4.30469	89.854	-577.521113414	3.806130739	12.347114	0.004856932	16.15810167
517	4.400	12	4.34908	89.622	-577.521194558	3.602456378	12.72472667	0.032556667	16.35973971
518	4.425	12	4.39354	89.387	-577.521272564	3.40665851	13.08243269	0.085620406	16.5747116
519	4.450	12	4.43804	89.151	-577.521347451	3.218689444	13.42063377	0.164237268	16.80356048
520	4.475	12	4.48260	88.913	-577.521419243	3.038488939	13.74017668	0.269225021	17.04789065
521	4.500	12	4.52721	88.673	-577.521487965	2.865994245	14.04170874	0.401234416	17.3089374
522	4.525	12	4.57187	88.432	-577.521553646	2.701132571	14.32597434	0.560206894	17.58731381
523	4.550	12	4.61658	88.188	-577.521616312	2.543838655	14.59372716	0.748122504	17.88568832
524	4.575	12	4.66135	87.942	-577.521675991	2.394042216	14.84577664	0.965043907	18.20486276
525	4.600	12	4.70618	87.694	-577.521732707	2.251683015	15.08286236	1.211643726	18.54618911
526	4.625	12	4.75106	87.444	-577.521786484	2.116700809	15.30566623	1.488600056	18.91096709
527	4.650	12	4.79601	87.192	-577.521837341	1.989047908	15.51500344	1.796596457	19.30064781
528	4.675	12	4.84101	86.938	-577.521885293	1.868686662	15.71147928	2.13632196	19.7164879
529	4.700	12	4.88608	86.681	-577.521930351	1.755589459	15.89585972	2.509983328	20.16143251
530	4.725	12	4.93122	86.423	-577.521972523	1.649736221	16.06879358	2.915373571	20.63390337
531	4.750	12	4.97642	86.162	-577.522011810	1.551124437	16.23087245	3.356342505	21.13833939
532	4.775	12	5.02168	85.899	-577.522048211	1.459756617	16.38270574	3.832091503	21.67455386
533	4.800	12	5.06700	85.633	-577.522081723	1.37564029	16.52487779	4.345329519	22.2458476
534	4.800	13	5.07428	85.420	-577.521986325	1.615092704	16.54683615	4.779553069	22.94148192
535	4.775	13	5.02889	85.675	-577.521950062	1.70611414	16.4059684	4.262148289	22.37423083
536	4.750	13	4.98386	85.934	-577.521912118	1.801354946	16.25653327	3.766960625	21.82484884
537	4.725	13	4.93885	86.191	-577.521871223	1.904002868	16.09691334	3.305812956	21.30672917
538	4.700	13	4.89390	86.445	-577.521827442	2.013894754	15.92664009	2.879622393	20.82015724
539	4.675	13	4.84903	86.696	-577.521780770	2.131043154	15.74517606	2.48734719	20.36356641
540	4.650	13	4.80423	86.945	-577.521731201	2.255463129	15.55184926	2.126565487	19.93387787
541	4.625	13	4.75949	87.192	-577.521678720	2.387192328	15.34595593	1.796596457	19.52974472
542	4.600	13	4.71481	87.436	-577.521623321	2.526245813	15.12681158	1.497932949	19.15099034
543	4.575	13	4.67019	87.678	-577.521564978	2.672688843	14.89371422	1.228515847	18.79491891
544	4.550	13	4.62563	87.919	-577.521503670	2.82657413	14.64594761	0.986734908	18.45925664
545	4.525	13	4.58113	88.156	-577.521439369	2.987971955	14.3827852	0.774779579	18.14553673
546	4.500	13	4.53668	88.392	-577.521372048	3.156950088	14.10343044	0.589153444	17.84953398
547	4.475	13	4.49229	88.626	-577.521301678	3.333581322	13.80720921	0.430159776	17.57095031
548	4.450	13	4.44795	88.858	-577.521228232	3.517933426	13.49332552	0.297158762	17.3084177
549	4.425	13	4.40366	89.088	-577.521151683	3.710074172	13.1610607	0.189516056	17.06065093
550	4.400	13	4.35944	89.316	-577.521072006	3.91006631	12.80988672	0.106602781	16.82655581
551	4.375	13	4.31528	89.542	-577.520989181	4.117960042	12.43909401	0.047795531	16.60484958
552	4.350	13	4.27118	89.767	-577.520903193	4.333793017	12.04810252	0.012369957	16.3942655
553	4.325	13	4.22714	89.989	-577.520814031	4.557592847	11.63640707	2.75703E-05	16.19402748
554	4.300	13	4.18318	90.210	-577.520721691	4.789369571	11.20380057	0.010048354	16.0032185
555	4.275	13	4.13930	90.429	-577.520626174	5.02912068	10.75002587	0.041934447	15.821081
556	4.250	13	4.09549	90.646	-577.520527480	5.276846173	10.2748661	0.095087049	15.64679932

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
557	4.225	13	4.05178	90.861	-577.520425607	5.53255107	9.778733149	0.168912829	15.48019705
558	4.200	13	4.00816	91.074	-577.520320537	5.796280553	9.261838668	0.262823924	15.32094314
559	4.175	13	3.96464	91.284	-577.520212242	6.068104901	8.724893932	0.375652583	15.16865142
560	4.150	13	3.92123	91.493	-577.520100680	6.348129537	8.168947751	0.507897351	15.02497464
561	4.125	13	3.87792	91.700	-577.519985793	6.636500043	7.595173202	0.658497567	14.89017081
562	4.100	13	3.83473	91.904	-577.519867515	6.933382082	7.005583982	0.826019348	14.76498541
563	4.075	13	3.79165	92.106	-577.519745764	7.238981474	6.402314362	1.010585507	14.65188134
564	4.050	13	3.74869	92.306	-577.519620459	7.553501536	5.788375382	1.211643726	14.55352064
565	4.025	13	3.70586	92.503	-577.519491517	7.877150597	5.167485208	1.427506292	14.4721421
566	4.000	13	3.66315	92.697	-577.519358862	8.210119423	4.543877923	1.657365236	14.41136258
567	3.975	13	3.62057	92.888	-577.519222427	8.552576185	3.92300529	1.90042489	14.37600636
568	3.950	13	3.57813	93.077	-577.519082162	8.904646384	3.311382071	2.15730388	14.37333234
569	3.925	13	3.53582	93.262	-577.518938031	9.266420383	2.716451515	2.424511484	14.40738338
570	3.900	13	3.49365	93.445	-577.518790019	9.637935831	2.147335172	2.704174945	14.48944595
571	3.875	13	3.45163	93.623	-577.518638128	10.01918771	1.61471951	2.990838759	14.62474598
572	3.850	13	3.40977	93.799	-577.518482373	10.41013837	1.13105218	3.288477836	14.82966838
573	3.825	13	3.36806	93.970	-577.518322783	10.81071501	0.710572338	3.591181421	15.11246877
574	3.800	13	3.32651	94.138	-577.518159378	11.22086744	0.37003955	3.901551148	15.49245814
575	3.800	14	3.34528	93.623	-577.517980770	11.66917995	0.512968552	2.990838759	15.17298727
576	3.825	14	3.38623	93.473	-577.518146033	11.25436387	0.88514845	2.748311143	14.88782347
577	3.850	14	3.42743	93.312	-577.518307493	10.84909346	1.32848731	2.499407037	14.67698781
578	3.875	14	3.46888	93.148	-577.518465125	10.45343147	1.82843282	2.258009576	14.53987386
579	3.900	14	3.51050	92.979	-577.518618913	10.06741805	2.371229802	2.022075366	14.46072322
580	3.925	14	3.55229	92.806	-577.518768833	9.691113454	2.945731835	1.794038115	14.4308834
581	3.950	14	3.59423	92.629	-577.518914882	9.324525206	3.542101517	1.57484387	14.44147059
582	3.975	14	3.63634	92.449	-577.519057077	8.967610637	4.152476011	1.366576356	14.486663
583	4.000	14	3.67858	92.266	-577.519195450	8.620289426	4.76937369	1.169973818	14.55963693
584	4.025	14	3.72096	92.080	-577.519330051	8.28243607	5.387136719	0.985786808	14.6553596
585	4.050	14	3.76348	91.890	-577.519460944	7.953889928	6.000930067	0.813916664	14.76873666
586	4.075	14	3.80612	91.699	-577.519588202	7.634467767	6.606479018	0.657723092	14.89866988
587	4.100	14	3.84890	91.504	-577.519711903	7.323973803	7.200815613	0.515409008	15.04019842
588	4.125	14	3.89179	91.307	-577.519832128	7.022204726	7.780913538	0.389231076	15.19234934
589	4.150	14	3.93481	91.108	-577.519948952	6.72897228	8.344988877	0.279727944	15.3536891
590	4.175	14	3.97794	90.907	-577.520062441	6.444110804	8.89119891	0.187443725	15.52275344
591	4.200	14	4.02119	90.703	-577.520172652	6.167477226	9.418501571	0.112607413	15.69858621
592	4.225	14	4.06453	90.497	-577.520279626	5.898968635	9.925722851	0.056281947	15.88097343
593	4.250	14	4.10798	90.289	-577.520383392	5.63851224	10.41258921	0.01903058	16.07013203
594	4.275	14	4.15152	90.079	-577.520483967	5.386065369	10.87861603	0.001422036	16.26610344
595	4.300	14	4.19514	89.867	-577.520581354	5.141620493	11.32366457	0.004030506	16.46931557
596	4.325	14	4.23885	89.653	-577.520675552	4.905180122	11.74797576	0.027435652	16.68059154
597	4.350	14	4.28263	89.437	-577.520766563	4.676739236	12.15164128	0.0722226	16.90060312
598	4.375	14	4.32649	89.219	-577.520854391	4.456287794	12.53515907	0.13898195	17.13042882
599	4.400	14	4.37040	89.000	-577.520939046	4.243800696	12.89877564	0.227853829	17.37043017

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
600	4.425	14	4.41439	88.778	-577.521020546	4.039232762	13.24331729	0.340250478	17.62280053
601	4.450	14	4.45843	88.555	-577.521098911	3.842533791	13.56917852	0.475764492	17.8874768
602	4.475	14	4.50253	88.329	-577.521174166	3.653641032	13.87711307	0.636222805	18.16697691
603	4.500	14	4.54670	88.101	-577.521246340	3.472481694	14.16788306	0.821686708	18.46205146
604	4.525	14	4.59092	87.872	-577.521315459	3.298990516	14.44207008	1.031809636	18.77287023
605	4.550	14	4.63520	87.640	-577.521381552	3.133094706	14.70046149	1.269054689	19.10261089
606	4.575	14	4.67954	87.406	-577.521444648	2.974721475	14.94377636	1.533191051	19.45168889
607	4.600	14	4.72394	87.169	-577.521504772	2.82380807	15.17272749	1.826148415	19.82268397
608	4.625	14	4.76841	86.930	-577.521561949	2.680291742	15.38806369	2.147499557	20.21585499
609	4.650	14	4.81294	86.689	-577.521616199	2.544122289	15.59041954	2.497897961	20.63243979
610	4.675	14	4.85755	86.446	-577.521667539	2.415257041	15.78054774	2.87800258	21.07380736
611	4.700	14	4.90222	86.200	-577.521715982	2.293663367	15.9590057	3.290209298	21.54287836
612	4.725	14	4.94696	85.951	-577.521761538	2.179316167	16.12645923	3.73552705	22.04130245
613	4.750	14	4.99176	85.700	-577.521804210	2.07220791	16.28347425	4.213017307	22.56869947
614	4.775	14	5.03665	85.447	-577.521843999	1.972336088	16.43072938	4.723366365	23.12643184
615	4.800	14	5.08160	85.191	-577.521880902	1.87970823	16.56867642	5.269457258	23.71784191
616	4.800	15	5.08986	84.943	-577.521768675	2.16140204	16.59303685	5.826962717	24.5814016
617	4.775	15	5.04498	85.191	-577.521729783	2.25902236	16.45699383	5.269457258	23.98547345
618	4.750	15	5.00032	85.440	-577.521688093	2.363665761	16.31231357	4.737901389	23.41388072
619	4.725	15	4.95571	85.686	-577.521643478	2.475651017	16.15794476	4.240495568	22.87409135
620	4.700	15	4.91119	85.930	-577.521595985	2.594860157	15.99346257	3.7743759	22.36269863
621	4.675	15	4.86673	86.170	-577.521545601	2.721325811	15.81817379	3.342365039	21.88186464
622	4.650	15	4.82235	86.408	-577.521492318	2.855068059	15.63154994	2.939875832	21.42649383
623	4.625	15	4.77805	86.643	-577.521436122	2.996122042	15.4329714	2.567787111	20.99688056
624	4.600	15	4.73381	86.876	-577.521376998	3.14452541	15.22170203	2.223711195	20.58993864
625	4.575	15	4.68964	87.106	-577.521314923	3.300335895	14.99712188	1.908329595	20.20578737
626	4.550	15	4.64554	87.334	-577.521249875	3.463608717	14.75855359	1.619483853	19.84164616
627	4.525	15	4.60150	87.559	-577.521181826	3.634414156	14.50525004	1.357662714	19.49732691
628	4.500	15	4.55753	87.782	-577.521110748	3.812822495	14.23656914	1.120932383	19.17032402
629	4.475	15	4.51361	88.003	-577.521036612	3.998906524	13.95168189	0.908683123	18.85927153
630	4.450	15	4.46976	88.222	-577.520959389	4.192739034	13.65001604	0.720310665	18.56306574
631	4.425	15	4.42598	88.439	-577.520879051	4.394390306	13.3308942	0.555216211	18.28050072
632	4.400	15	4.38226	88.653	-577.520795572	4.603925601	12.9935824	0.413420039	18.01092804
633	4.375	15	4.33861	88.866	-577.520708930	4.821400141	12.63753021	0.293009999	17.75194035
634	4.350	15	4.29503	89.076	-577.520619108	5.046856594	12.26216351	0.194536131	17.50355624
635	4.325	15	4.25153	89.285	-577.520526093	5.280327593	11.86706403	0.116484574	17.2638762
636	4.300	15	4.20811	89.491	-577.520429881	5.521823176	11.4518158	0.059032598	17.03267158
637	4.275	15	4.16477	89.696	-577.520330471	5.771345855	11.01610565	0.02105734	16.80850884
638	4.250	15	4.12152	89.898	-577.520227863	6.028895629	10.55985583	0.002370591	16.59112205
639	4.225	15	4.07837	90.099	-577.520122053	6.294482538	10.08316471	0.002233195	16.37988044
640	4.200	15	4.03533	90.297	-577.520013025	6.568146743	9.586339463	0.020098758	16.17458496
641	4.175	15	3.99240	90.493	-577.519900752	6.849956015	9.069810299	0.055379645	15.97514596
642	4.150	15	3.94957	90.687	-577.519785189	7.140023305	8.534148377	0.107539944	15.78171163

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
643	4.125	15	3.90688	90.878	-577.519666275	7.438501726	7.980883042	0.175648871	15.59503364
644	4.100	15	3.86430	91.067	-577.519543958	7.7455218	7.411032218	0.259409078	15.4159631
645	4.075	15	3.82186	91.254	-577.519418159	8.061281818	6.826835335	0.358303793	15.24642095
646	4.050	15	3.77956	91.437	-577.519288799	8.385980075	6.230647902	0.470511094	15.08713907
647	4.025	15	3.73739	91.618	-577.519155806	8.719797293	5.625257145	0.596504009	14.94155845
648	4.000	15	3.69537	91.795	-577.519019106	9.062919214	5.014547591	0.734150735	14.81161754
649	3.975	15	3.65351	91.969	-577.518878640	9.415493931	4.403030637	0.883380411	14.70190498
650	3.950	15	3.61180	92.140	-577.518734365	9.777629375	3.795793702	1.043479397	14.61690247
651	3.925	15	3.57024	92.307	-577.518586247	10.14941089	3.199063318	1.212694816	14.56116902
652	3.900	15	3.52885	92.470	-577.518434275	10.53086608	2.6204754	1.390113428	14.54145491
653	3.875	15	3.48763	92.630	-577.518278451	10.92198993	2.068641658	1.576042153	14.56667374
654	3.850	15	3.44657	92.785	-577.518118792	11.32273977	1.553491074	1.767285569	14.64351641
655	3.825	15	3.40569	92.937	-577.517955322	11.73305535	1.086953758	1.96546007	14.78546918
656	3.800	15	3.36498	93.084	-577.517788059	12.1528915	0.682415585	2.167130532	15.00243762
657	3.800	16	3.38610	92.512	-577.517580943	12.67276012	0.883850055	1.437790475	14.99440065
658	3.825	16	3.42618	92.384	-577.517750381	12.24746464	1.314177207	1.294997214	14.85663906
659	3.850	16	3.46645	92.244	-577.517916036	11.83166462	1.79788282	1.147366161	14.77691361
660	3.875	16	3.50706	92.100	-577.518077896	11.4253902	2.32510902	1.004835388	14.75533461
661	3.900	16	3.54784	91.951	-577.518235932	11.02871415	2.883459817	0.867303044	14.77947701
662	3.925	16	3.58881	91.798	-577.518390126	10.64168166	3.464221287	0.736606771	14.84250972
663	3.950	16	3.62997	91.640	-577.518540476	10.26429774	4.059690082	0.61283566	14.93682349
664	3.975	16	3.67131	91.478	-577.518686995	9.89652978	4.663134014	0.497743045	15.05740684
665	4.000	16	3.71281	91.313	-577.518829713	9.538302463	5.268665841	0.392812939	15.19978124
666	4.025	16	3.75446	91.144	-577.518968672	9.18951037	5.871433318	0.298200509	15.3591442
667	4.050	16	3.79627	90.972	-577.519103933	8.85000039	6.467658594	0.215272652	15.53293164
668	4.075	16	3.83822	90.798	-577.519235559	8.519614392	7.05382457	0.14509823	15.71853719
669	4.100	16	3.88032	90.620	-577.519363623	8.198169142	7.627443076	0.087587012	15.91319923
670	4.125	16	3.92255	90.440	-577.519488199	7.885478897	8.186142413	0.044112501	16.11573381
671	4.150	16	3.96492	90.257	-577.519609357	7.581367955	8.72841488	0.015049518	16.32483235
672	4.175	16	4.00741	90.071	-577.519727162	7.285673164	9.252763142	0.001148611	16.53958492
673	4.200	16	4.05003	89.883	-577.519841668	6.998258982	9.758412681	0.003119091	16.75979075
674	4.225	16	4.09276	89.693	-577.519952918	6.719017477	10.24452347	0.021474996	16.98501594
675	4.250	16	4.13560	89.500	-577.520060941	6.447875858	10.71075197	0.056963457	17.21559129
676	4.275	16	4.17855	89.305	-577.520165752	6.184796475	11.15696095	0.110059096	17.45181652
677	4.300	16	4.22158	89.109	-577.520267356	5.929766777	11.58289605	0.180888826	17.69355165
678	4.325	16	4.26472	88.910	-577.520365751	5.682791785	11.9890542	0.270713135	17.94255912
679	4.350	16	4.30793	88.709	-577.520460940	5.443863968	12.37538241	0.379759648	18.19900603
680	4.375	16	4.35123	88.505	-577.520552929	5.212968267	12.74249119	0.509259005	18.46471846
681	4.400	16	4.39460	88.300	-577.520641730	4.99007456	13.09071638	0.658497567	18.73928851
682	4.425	16	4.43804	88.093	-577.520727353	4.775157747	13.42063377	0.828624401	19.02441591
683	4.450	16	4.48156	87.883	-577.520809837	4.568119938	13.73293088	1.021170001	19.32222082
684	4.475	16	4.52514	87.671	-577.520889200	4.368915951	14.02811208	1.235934084	19.63296212
685	4.500	16	4.56880	87.457	-577.520965471	4.177472995	14.30698055	1.473496309	19.95794986

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
686	4.525	16	4.61252	87.241	-577.521038680	3.99371577	14.57008708	1.734441806	20.29824465
687	4.550	16	4.65631	87.022	-577.521108856	3.817571483	14.81817963	2.020718041	20.65646916
688	4.575	16	4.70017	86.800	-577.521176029	3.648964835	15.05193826	2.333223214	21.03412631
689	4.600	16	4.74410	86.576	-577.521240224	3.487833074	15.27203593	2.671307258	21.43117626
690	4.625	16	4.78810	86.350	-577.521301468	3.334108429	15.47913456	3.035582643	21.84882564
691	4.650	16	4.83218	86.120	-577.521359782	3.18773819	15.67392459	3.430202691	22.29186547
692	4.675	16	4.87633	85.888	-577.521415185	3.048674665	15.85698873	3.852676501	22.7583399
693	4.700	16	4.92056	85.654	-577.521467690	2.916885225	16.0289771	4.303638421	23.24950074
694	4.725	16	4.96487	85.416	-577.521517307	2.792344769	16.19047477	4.787905279	23.77072482
695	4.750	16	5.00925	85.176	-577.521564041	2.675040746	16.34201327	5.302380997	24.31943501
696	4.775	16	5.05372	84.933	-577.521607893	2.564970648	16.48420401	5.850030639	24.89920529
697	4.800	16	5.09828	84.688	-577.521648861	2.462139493	16.61756214	6.429429888	25.50913152
698	4.800	17	5.10763	84.407	-577.521521469	2.781897999	16.64443745	7.127643517	26.55397896
699	4.775	17	5.06318	84.644	-577.521478238	2.890409366	16.51326015	6.536382653	25.94005216
700	4.750	17	5.01891	84.883	-577.521432110	3.006192306	16.37370223	5.966053809	25.34594834
701	4.725	17	4.97473	85.118	-577.521383083	3.129251841	16.22500427	5.430650855	24.78490697
702	4.700	17	4.93064	85.350	-577.521331176	3.25954028	16.06664315	4.926769428	24.25295286
703	4.675	17	4.88664	85.580	-577.521276376	3.397090253	15.89807561	4.451443554	23.74660942
704	4.650	17	4.84273	85.805	-577.521218666	3.54194443	15.71873898	4.009777388	23.2704608
705	4.625	17	4.79890	86.029	-577.521158049	3.694095282	15.52800734	3.592990808	22.81509343
706	4.600	17	4.75515	86.249	-577.521094499	3.85360807	15.32527407	3.205903609	22.38478575
707	4.575	17	4.71148	86.466	-577.521027995	4.020535504	15.1099166	2.845702022	21.97615412
708	4.550	17	4.66788	86.681	-577.520958514	4.194935316	14.88124466	2.509983328	21.58616331
709	4.525	17	4.62436	86.893	-577.520886026	4.376882805	14.6386588	2.199575322	21.21511693
710	4.500	17	4.58091	87.102	-577.520810504	4.566445744	14.3814438	1.913608513	20.86149806
711	4.475	17	4.53753	87.309	-577.520731916	4.763704453	14.10893193	1.649999177	20.52263556
712	4.450	17	4.49422	87.514	-577.520650232	4.968734234	13.82045752	1.408181326	20.19737308
713	4.425	17	4.45099	87.716	-577.520565421	5.181612897	13.51543619	1.188635047	19.88568413
714	4.400	17	4.40784	87.916	-577.520477457	5.402405704	13.19324013	0.989581941	19.58522778
715	4.375	17	4.36477	88.113	-577.520386314	5.631177915	12.85326852	0.811334853	19.29578129
716	4.350	17	4.32177	88.309	-577.520291976	5.867969691	12.49487294	0.651543696	19.01438632
717	4.325	17	4.27887	88.502	-577.520194428	6.112818683	12.11779842	0.511304905	18.74192201
718	4.300	17	4.23606	88.693	-577.520093663	6.36574246	11.72153258	0.389231076	18.47650612
719	4.275	17	4.19334	88.881	-577.519989681	6.626741024	11.30572881	0.285309679	18.21777951
720	4.250	17	4.15074	89.067	-577.519882483	6.895811863	10.87045947	0.198344252	17.96461559
721	4.225	17	4.10823	89.252	-577.519772064	7.172967528	10.41532749	0.127485129	17.71578015
722	4.200	17	4.06585	89.433	-577.519658409	7.458245669	9.940834022	0.0732525	17.47233219
723	4.175	17	4.02359	89.612	-577.519541491	7.751714058	9.447148552	0.034302027	17.23316464
724	4.150	17	3.98145	89.789	-577.519421267	8.053480626	8.934766361	0.01014428	16.99839127
725	4.125	17	3.93945	89.963	-577.519297683	8.363680915	8.404700296	0.000311932	16.76869314
726	4.100	17	3.89759	90.135	-577.519170675	8.682475568	7.858037522	0.004152636	16.54466573
727	4.075	17	3.85587	90.303	-577.519040175	9.010035266	7.296217884	0.020919032	16.32717218
728	4.050	17	3.81431	90.469	-577.518906111	9.346540732	6.721369985	0.050118956	16.11802967

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
729	4.025	17	3.77290	90.631	-577.518768414	9.692165159	6.135688815	0.090722509	15.91857648
730	4.000	17	3.73166	90.790	-577.518627022	10.04706417	5.542330686	0.142203575	15.73159843
731	3.975	17	3.69058	90.945	-577.518481881	10.4113733	4.944641153	0.203479166	15.55949362
732	3.950	17	3.64968	91.096	-577.518332954	10.78518544	4.347097383	0.273701666	15.40598448
733	3.925	17	3.60896	91.244	-577.518180209	11.16858088	3.754673919	0.352612004	15.27586681
734	3.900	17	3.56842	91.387	-577.518023638	11.56157973	3.173232788	0.438338134	15.17315065
735	3.875	17	3.52808	91.526	-577.517863243	11.96417696	2.609914202	0.530597744	15.1046889
736	3.850	17	3.48792	91.660	-577.517699039	12.37633491	2.072415904	0.627874013	15.07662482
737	3.825	17	3.44795	91.790	-577.517531049	12.79799585	1.570120739	0.730066455	15.09818305
738	3.800	17	3.40817	91.916	-577.517359286	13.22912717	1.11368812	0.836464168	15.17927946
739	3.800	18	3.43153	91.289	-577.517122754	13.822831	1.375766438	0.378583923	15.57718136
740	3.825	18	3.47066	91.185	-577.517297029	13.38539448	1.850899242	0.319958044	15.55625176
741	3.850	18	3.50990	91.069	-577.517467547	12.95738816	2.363170964	0.26038247	15.58094159
742	3.875	18	3.54960	90.945	-577.517634287	12.53886476	2.908061518	0.203479166	15.65040544
743	3.900	18	3.58947	90.818	-577.517797232	12.12986694	3.473694117	0.152462466	15.75602352
744	3.925	18	3.62954	90.685	-577.517956366	11.73043487	4.053430947	0.106914713	15.89078053
745	3.950	18	3.66983	90.548	-577.518111686	11.34057608	4.641504012	0.068425416	16.05050551
746	3.975	18	3.71031	90.406	-577.518263203	10.96026296	5.232285018	0.037558514	16.23010649
747	4.000	18	3.75097	90.260	-577.518410946	10.58942271	5.821215246	0.015402919	16.42604087
748	4.025	18	3.79181	90.111	-577.518554950	10.22796748	6.404579784	0.002807387	16.63535465
749	4.050	18	3.83281	89.959	-577.518695269	9.875761742	6.979002091	0.000383022	16.85514686
750	4.075	18	3.87398	89.803	-577.518831959	9.532664922	7.542080312	0.008842779	17.08358801
751	4.100	18	3.91530	89.644	-577.518965087	9.198508849	8.091483431	0.028877283	17.31886956
752	4.125	18	3.95678	89.482	-577.519094720	8.873125352	8.625711129	0.061138651	17.55997513
753	4.150	18	3.99840	89.317	-577.519220927	8.556341239	9.14324395	0.106291305	17.80587649
754	4.175	18	4.04017	89.150	-577.519343768	8.248005906	9.64326707	0.164624392	18.05589737
755	4.200	18	4.08207	88.980	-577.519463298	7.947981303	10.12488177	0.237059124	18.3099222
756	4.225	18	4.12410	88.807	-577.519579557	7.656167028	10.58767696	0.324292735	18.56813672
757	4.250	18	4.16625	88.632	-577.519692573	7.372492799	11.03133795	0.426411125	18.83024188
758	4.275	18	4.20853	88.454	-577.519802359	7.096925987	11.45593384	0.544597084	19.09745691
759	4.300	18	4.25091	88.274	-577.519908918	6.829459061	11.86128258	0.678793875	19.36953551
760	4.325	18	4.29340	88.091	-577.520012251	6.570089511	12.24773014	0.830363382	19.64818303
761	4.350	18	4.33599	87.906	-577.520112358	6.318817337	12.61553118	0.999101674	19.93345019
762	4.375	18	4.37867	87.719	-577.520209246	6.075624969	12.96503533	1.185514588	20.22617489
763	4.400	18	4.42144	87.529	-577.520302928	5.840479777	13.29674546	1.391239254	20.52846449
764	4.425	18	4.46430	87.337	-577.520393424	5.613331559	13.61121059	1.615841154	20.8403833
765	4.450	18	4.50724	87.142	-577.520480758	5.394120075	13.90894669	1.861147447	21.16421421
766	4.475	18	4.55026	86.945	-577.520564958	5.182775043	14.19057273	2.126565487	21.49991326
767	4.500	18	4.59336	86.745	-577.520646055	4.979218654	14.45672243	2.41411702	21.85005811
768	4.525	18	4.63654	86.542	-577.520724082	4.783368075	14.708037	2.724622319	22.2160274
769	4.550	18	4.67980	86.337	-577.520799069	4.595148006	14.94515911	3.057244479	22.5975516
770	4.575	18	4.72314	86.128	-577.520871047	4.414480634	15.16872785	3.416072107	22.99928059
771	4.600	18	4.76656	85.917	-577.520940043	4.241298191	15.37937456	3.798525899	23.41919865

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
772	4.625	18	4.81006	85.704	-577.521006084	4.075532903	15.57771952	4.205182781	23.85843521
773	4.650	18	4.85365	85.487	-577.521069190	3.917134571	15.76441064	4.640737452	24.32228266
774	4.675	18	4.89733	85.267	-577.521129380	3.766055504	15.9400307	5.104219484	24.81030569
775	4.700	18	4.94109	85.044	-577.521186667	3.622263072	16.10510915	5.596531177	25.3239034
776	4.725	18	4.98495	84.818	-577.521241059	3.485737194	16.26026914	6.118587137	25.86459347
777	4.750	18	5.02890	84.589	-577.521292558	3.35647285	16.40600049	6.671314273	26.43378762
778	4.775	18	5.07295	84.357	-577.521341163	3.23447255	16.54284228	7.255651798	27.03296663
779	4.800	18	5.11710	84.122	-577.521386867	3.119753865	16.67127762	7.872551231	27.66358272
780	4.800	19	5.12766	83.808	-577.521244832	3.476266828	16.7007622	8.736112688	28.91314172
781	4.775	19	5.08363	84.033	-577.521196543	3.597473957	16.57469114	8.112755878	28.28492097
782	4.750	19	5.03973	84.263	-577.521145326	3.72603047	16.44047846	7.499391597	27.66590053
783	4.725	19	4.99600	84.486	-577.521091197	3.861896209	16.29780471	6.927712491	27.08741341
784	4.700	19	4.95236	84.707	-577.521034162	4.005056112	16.14593808	6.383518481	26.53451267
785	4.675	19	4.90883	84.924	-577.520974220	4.15551269	15.98444069	5.870830731	26.01078411
786	4.650	19	4.86540	85.138	-577.520911363	4.313286023	15.81275351	5.386246701	25.51228623
787	4.625	19	4.82206	85.348	-577.520845582	4.478398701	15.63029068	4.931008421	25.0396978
788	4.600	19	4.77882	85.556	-577.520776858	4.650898415	15.43653181	4.499916267	24.5873465
789	4.575	19	4.73567	85.760	-577.520705173	4.830830346	15.2308548	4.096265005	24.15795015
790	4.550	19	4.69261	85.961	-577.520630501	5.018259754	15.0126652	3.717098232	23.74802318
791	4.525	19	4.64963	86.159	-577.520552815	5.213254411	14.78130248	3.361591573	23.35614847
792	4.500	19	4.60673	86.355	-577.520472084	5.415892127	14.5361439	3.027271675	22.9793077
793	4.475	19	4.56392	86.547	-577.520388275	5.626255734	14.2766244	2.71674883	22.61962897
794	4.450	19	4.52120	86.737	-577.520301356	5.844425553	14.0021276	2.42599823	22.27255139
795	4.425	19	4.47856	86.924	-577.520211295	6.070481906	13.71197347	2.155901895	21.93835727
796	4.400	19	4.43601	87.109	-577.520118063	6.304497582	13.40562685	1.904375192	21.61449962
797	4.375	19	4.39356	87.290	-577.520021634	6.546537843	13.08258909	1.673381309	21.30250824
798	4.350	19	4.35120	87.469	-577.519921988	6.796652891	12.74224364	1.459622745	20.99851928
799	4.325	19	4.30895	87.646	-577.519819113	7.054872844	12.38425848	1.262610071	20.7017414
800	4.300	19	4.26680	87.820	-577.519713000	7.321220294	12.00811663	1.082852539	20.41218946
801	4.275	19	4.22477	87.991	-577.519603651	7.595690221	11.61363991	0.919636512	20.12896665
802	4.250	19	4.18286	88.159	-577.519491066	7.878282624	11.20057114	0.772260655	19.85111442
803	4.225	19	4.14108	88.325	-577.519375244	8.169000013	10.76886362	0.6392724	19.57713603
804	4.200	19	4.09943	88.489	-577.519256173	8.46787251	10.31850563	0.520217863	19.306596
805	4.175	19	4.05792	88.649	-577.519133826	8.774967884	9.84975153	0.415879037	19.04059845
806	4.150	19	4.01656	88.807	-577.519008164	9.090384028	9.363052945	0.324292735	18.77772971
807	4.125	19	3.97535	88.962	-577.518879137	9.414246443	8.858964316	0.245499741	18.5187105
808	4.100	19	3.93429	89.114	-577.518746682	9.746713261	8.338283085	0.178864345	18.26386069
809	4.075	19	3.89340	89.262	-577.518610734	10.08794764	7.802354792	0.124099221	18.01440165
810	4.050	19	3.85268	89.408	-577.518471227	10.43811523	7.252607065	0.079854564	17.77057686
811	4.025	19	3.81213	89.550	-577.518328099	10.79737166	6.690837123	0.0461404	17.53434918
812	4.000	19	3.77175	89.688	-577.518181294	11.1658575	6.11926492	0.022180203	17.30730262
813	3.975	19	3.73157	89.823	-577.518030764	11.54369321	5.541027114	0.007138433	17.09185876
814	3.950	19	3.69158	89.953	-577.517876475	11.93096416	4.959238511	0.000503329	16.890706

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
815	3.925	19	3.65178	90.080	-577.517718402	12.32773308	4.377763394	0.001458265	16.70695474
816	3.900	19	3.61218	90.201	-577.517556535	12.73402508	3.8012986	0.009205523	16.5445292
817	3.875	19	3.57279	90.319	-577.517390871	13.14984768	3.235304895	0.023186634	16.40833921
818	3.850	19	3.53361	90.431	-577.517221426	13.57516073	2.685947914	0.042326355	16.303435
819	3.825	19	3.49464	90.539	-577.517048218	14.00991905	2.160344714	0.066196322	16.23646008
820	3.800	19	3.45589	90.642	-577.516871257	14.45409753	1.666797137	0.093913146	16.21480781
821	3.800	20	3.48124	89.968	-577.516604454	15.12378266	1.98591977	0.000233322	17.10993575
822	3.825	20	3.51939	89.889	-577.516784256	14.67247317	2.491328277	0.002807387	17.16660883
823	3.850	20	3.55758	89.794	-577.516960382	14.23039057	3.020046479	0.009669205	17.26010625
824	3.875	20	3.59629	89.692	-577.517132734	13.79778084	3.571752621	0.021615126	17.39114859
825	3.900	20	3.63517	89.586	-577.517301323	13.37461638	4.135425287	0.039053235	17.54909491
826	3.925	20	3.67422	89.476	-577.517466138	12.9609248	4.705661848	0.062563193	17.72914984
827	3.950	20	3.71355	89.360	-577.517627168	12.5567337	5.27943113	0.093328929	17.92949376
828	3.975	20	3.75309	89.240	-577.517784430	12.16200042	5.851727516	0.131608372	18.14533631
829	4.000	20	3.79281	89.115	-577.517937947	11.77666723	6.418734763	0.178460816	18.3738628
830	4.025	20	3.83273	88.987	-577.518087755	11.40064375	6.97789386	0.233816536	18.61235415
831	4.050	20	3.87283	88.856	-577.518233898	11.03381956	7.526556523	0.298200509	18.85857659
832	4.075	20	3.91311	88.721	-577.518376429	10.67606162	8.062785251	0.372732636	19.11157951
833	4.100	20	3.95356	88.583	-577.518515408	10.32721933	8.584887558	0.457505198	19.36961208
834	4.125	20	3.99419	88.441	-577.518650898	9.98713455	9.091759866	0.553794403	19.63268882
835	4.150	20	4.03499	88.297	-577.518782962	9.655649155	9.58233039	0.660823727	19.89880327
836	4.175	20	4.07594	88.149	-577.518911660	9.332612542	10.05568093	0.780673018	20.16896649
837	4.200	20	4.11706	87.998	-577.519037042	9.017899208	10.51158078	0.91323906	20.44271905
838	4.225	20	4.15833	87.845	-577.519159145	8.711416283	10.94953218	1.05815888	20.71910734
839	4.250	20	4.19973	87.688	-577.519277991	8.413108544	11.36923432	1.2179571	21.00029997
840	4.275	20	4.24128	87.529	-577.519393592	8.122945873	11.77093626	1.391239254	21.28512139
841	4.300	20	4.28297	87.366	-577.519505949	7.840925758	12.15469396	1.580839843	21.57645956
842	4.325	20	4.32477	87.201	-577.519615057	7.56706075	12.52050581	1.78509827	21.87266483
843	4.350	20	4.36670	87.033	-577.519720916	7.301350849	12.8689052	2.00581754	22.17607359
844	4.375	20	4.40873	86.863	-577.519823534	7.043775975	13.20006938	2.242256902	22.48610226
845	4.400	20	4.45087	86.689	-577.519922921	6.794311027	13.51456507	2.497897961	22.80677405
846	4.425	20	4.49312	86.512	-577.520019100	6.552898274	13.81291084	2.7721025	23.13791162
847	4.450	20	4.53545	86.333	-577.520112096	6.319474966	14.09545827	3.063925153	23.47885839
848	4.475	20	4.57789	86.151	-577.520201937	6.093970822	14.36298924	3.375609141	23.83256921
849	4.500	20	4.62041	85.965	-577.520288657	5.8763005	14.61590686	3.709739465	24.20194682
850	4.525	20	4.66303	85.777	-577.520372290	5.66637866	14.85493258	4.063483447	24.58479469
851	4.550	20	4.70574	85.585	-577.520452867	5.464127489	15.08060725	4.441378111	24.98611285
852	4.575	20	4.74854	85.391	-577.520530421	5.269464157	15.29352816	4.840271785	25.40326411
853	4.600	20	4.79144	85.193	-577.520604977	5.082325913	15.49432984	5.265075173	25.84173093
854	4.625	20	4.83442	84.992	-577.520676562	4.902644986	15.68349688	5.714588626	26.30073049
855	4.650	20	4.87752	84.788	-577.520745193	4.730378705	15.86176257	6.189636518	26.78177779
856	4.675	20	4.92071	84.580	-577.520810886	4.56548691	16.02954169	6.693525236	27.28855383
857	4.700	20	4.96400	84.369	-577.520873649	4.407949521	16.18740393	7.22482591	27.82017936

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)^3**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
858	4.725	20	5.00741	84.155	-577.520933486	4.257756497	16.33592576	7.784403927	28.37808618
859	4.750	20	5.05094	83.937	-577.520990393	4.114917878	16.47558734	8.375899708	28.96640493
860	4.775	20	5.09458	83.716	-577.521044363	3.979451235	16.60682294	8.997641491	29.58391566
861	4.800	20	5.13833	83.492	-577.521095383	3.851389198	16.73008423	9.650535676	30.23200911
1b	3.800	22	3.52962	88.621	-577.516027068	16.57304231	2.631045044	0.433296184	19.63738354
2b	3.900	22	3.67670	88.401	-577.516749231	14.76038718	4.741902913	0.582576899	20.08486699
3b	4.000	22	3.83772	87.920	-577.517412382	13.0958543	7.046919487	0.985786808	21.12856059
4b	4.100	22	3.99711	87.442	-577.518016008	11.58073131	9.12748949	1.490930545	22.19915134
5b	4.200	22	4.15534	87.014	-577.518564743	10.2033867	10.91846131	2.031589403	23.15343741
6b	4.300	22	4.32021	86.412	-577.519059910	8.960499705	12.48150618	2.93333187	24.37533775
7b	4.400	22	4.48629	85.792	-577.519503313	7.847542213	13.76580481	4.034667912	25.64801493
8b	4.500	22	4.64780	85.200	-577.519894942	6.864539324	14.77113989	5.249752231	26.88543145
9b	4.600	22	4.82196	84.375	-577.520236242	6.007864037	15.62985633	7.209437573	28.84715794
10b	4.700	22	4.99601	83.524	-577.520528924	5.273221681	16.2978384	9.555865145	31.12692523
11b	4.800	22	5.16402	82.740	-577.520774822	4.656008848	16.79878777	12.0096285	33.46442512
12b	4.800	24	5.18602	82.040	-577.520419934	5.546790505	16.85555253	14.4371832	36.83952623
13b	4.700	24	5.01769	82.800	-577.520148977	6.226902329	16.36972505	11.81194252	34.4085699
14b	4.600	24	4.84386	83.623	-577.519828986	7.030091259	15.72349862	9.265933223	32.0195231
15b	4.500	24	4.68218	84.224	-577.519459464	7.957604781	14.95779321	7.601699561	30.51709755
16b	4.400	24	4.51836	84.836	-577.519039205	9.012470001	13.98331215	6.076154374	29.07193653
17b	4.300	24	4.35584	85.404	-577.518566462	10.19907195	12.78042021	4.813005657	27.79249782
18b	4.200	24	4.18962	85.993	-577.518040567	11.51908733	11.26854492	3.658432251	26.4460645
19b	4.100	24	4.04448	86.233	-577.517461880	12.97161253	9.693736083	3.23331169	25.89866031
20b	4.000	24	3.88970	86.554	-577.516828008	14.56265407	7.753042586	2.705745085	25.02144175
21b	3.900	24	3.73489	86.908	-577.516135692	16.30039216	5.589092941	2.178388334	24.06787343
22b	3.800	24	3.59381	87.049	-577.515383411	18.18864455	3.536059496	1.984242516	23.70894656
23b	3.800	26	3.65619	85.509	-577.514674319	19.968491	4.442179601	4.595602343	29.00627294
24b	3.900	26	3.79662	85.352	-577.515459559	17.99751033	6.472602968	4.922532258	29.39264555
25b	4.000	26	3.93670	85.257	-577.516186070	16.17394156	8.369338125	5.125810913	29.6690906
26b	4.100	26	4.08696	84.939	-577.516853697	14.49817376	10.17977385	5.836184417	30.51413203
27b	4.200	26	4.24154	84.570	-577.517465862	12.96161757	11.77338905	6.718247377	31.453254
28b	4.300	26	4.39839	84.165	-577.518024518	11.5593709	13.12024258	7.757790599	32.43740408
29b	4.400	26	4.55590	83.751	-577.518529542	10.29174248	14.22629578	8.897692269	33.41573052
30b	4.500	26	4.71706	83.216	-577.518981511	9.157284018	15.1381822	10.48643841	34.78190463
31b	4.600	26	4.88651	82.536	-577.519381120	8.154251042	15.89756137	12.69403214	36.74584455
32b	4.700	26	5.05219	81.823	-577.519730359	7.277648579	16.47946615	15.23506556	38.99218029
33b	4.800	26	5.21966	81.131	-577.520029455	6.526906852	16.93879654	17.92279106	41.38849445
34b	4.800	28	5.24671	80.407	-577.519602135	7.599495435	17.00273582	20.96839654	45.57062779
35b	4.700	28	5.07973	80.985	-577.519273641	8.424027201	16.56311964	18.51773199	43.50487883
36b	4.600	28	4.91598	81.650	-577.518891955	9.382072802	16.01167857	15.88653863	41.28029
37b	4.500	28	4.75045	82.261	-577.518458074	10.47112973	15.30273204	13.64664913	39.42051089
38b	4.400	28	4.59562	82.708	-577.517971258	11.69305542	14.47025017	12.11573183	38.27903741
39b	4.300	28	4.44530	82.986	-577.517430696	13.0498855	13.47397945	11.20954165	37.7334066

Step No.	C-C (Å)	Twist Angle	Ir-Ir (Å)	C-M-M (deg.)	Ligand E (Hartrees)	**Ligand E (x4) (kcal/mol)[3]**	**Morse E (kcal/mol)**	**A_{2U} E (x2) (kcal/mol)**	**Total E (kcal/mol)**
40b	4.200	28	4.28531	83.368	-577.516837089	14.53986044	12.17566949	10.02179159	36.73732152
41b	4.100	28	4.13325	83.673	-577.516188366	16.16817852	10.68572583	9.12120047	35.97510482
42b	4.000	28	3.98909	83.867	-577.515483522	17.93736234	9.029128449	8.57042308	35.53691386
43b	3.900	28	3.85246	83.906	-577.514720358	19.85293145	7.249596145	8.461770297	35.56429789
44b	3.800	28	3.71837	83.918	-577.513898465	21.91591247	5.349510483	8.428478119	35.69390107
45b	3.800	30	3.78596	82.269	-577.513053260	24.03740744	6.321639771	13.61844994	43.97749715
46b	3.900	30	3.91577	82.349	-577.513914570	21.87548834	8.097636098	13.33806213	43.31118656
47b	4.000	30	4.05022	82.316	-577.514717936	19.85901076	9.760620599	13.4533687	43.07300005
48b	4.100	30	4.19287	82.152	-577.515462288	17.99066044	11.30103952	14.03376891	43.32546887
49b	4.200	30	4.33917	81.912	-577.516150023	16.26442083	12.64222297	14.90522778	43.81187158
50b	4.300	30	4.48972	81.715	-577.516782820	14.67607758	13.78951476	15.64016598	44.10575832
51b	4.400	30	4.64431	81.372	-577.517360911	13.22504836	14.75168688	16.96198227	44.93871751
52b	4.500	30	4.79872	80.978	-577.517885152	11.90918458	15.52719898	18.54650059	45.98288415
53b	4.600	30	4.95424	80.604	-577.518355786	10.72787629	16.15268343	20.11603341	46.99659314
54b	4.700	30	5.11867	79.986	-577.518772174	9.682727424	16.67569076	22.84922668	49.20764486
55b	4.800	30	5.28477	79.276	-577.519133532	8.775705835	17.0883839	26.20414191	52.06823164

[1] Forster, L.S. in *Concepts of Inorganic Photochemistry*, Adamson, A.W.; Fleischauer, P.D.; eds., John Wiley and Sons: New York, 1978 and references therein.

[2] Additional ligand calculations were later done for twist angles = 22, 24, 26, 28, and 30° in an effort to expand the potential-energy surface. These structures (denoted by a 'b' in the Step Number column of Table S1) bring the total number of optimized structures to 916.

[3] This column shows relative deformational energy, with the ligand structure corresponding to a C---C distance of 4.8 Å and a 0° twist angle set to 0 kcal/mol.